



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:55 PM UTC

PDB ID : 4V4H / pdb\_00004v4h  
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with the antibiotic kasugamyin at 3.5Å resolution.  
Authors : Schuwirth, B.S.; Vila-Sanjurjo, A.; Cate, J.H.D.  
Deposited on : 2006-08-04  
Resolution : 3.46 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>.

---

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                                                             |

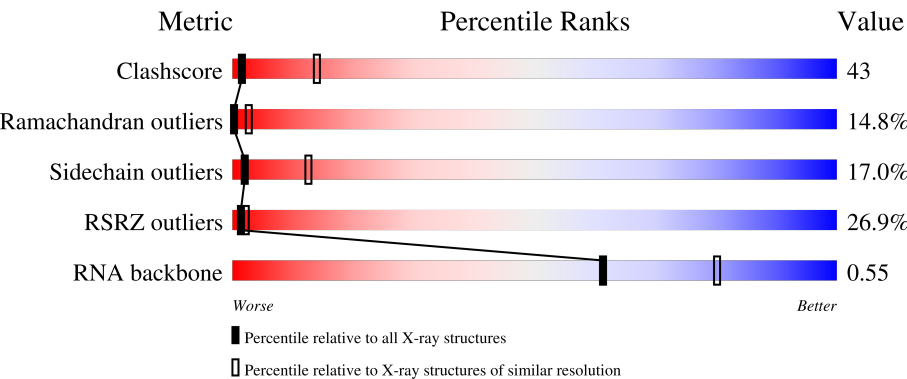
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.46 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 1128 (3.50-3.42)                                      |
| Ramachandran outliers | 187476                      | 1101 (3.50-3.42)                                      |
| Sidechain outliers    | 187428                      | 1102 (3.50-3.42)                                      |
| RSRZ outliers         | 180081                      | 1070 (3.50-3.42)                                      |
| RNA backbone          | 3983                        | 1186 (3.92-3.00)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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   | AA    | 1542   |                  |
| 1   | CA    | 1542   |                  |
| 2   | AC    | 233    |                  |
| 2   | CC    | 233    |                  |
| 3   | AD    | 206    |                  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | CD    | 206    |                  |
| 4   | AE    | 167    |                  |
| 4   | CE    | 167    |                  |
| 5   | AF    | 135    |                  |
| 5   | CF    | 135    |                  |
| 6   | AG    | 179    |                  |
| 6   | CG    | 179    |                  |
| 7   | AH    | 130    |                  |
| 7   | CH    | 130    |                  |
| 8   | AI    | 130    |                  |
| 8   | CI    | 130    |                  |
| 9   | AJ    | 103    |                  |
| 9   | CJ    | 103    |                  |
| 10  | AK    | 129    |                  |
| 10  | CK    | 129    |                  |
| 11  | AL    | 124    |                  |
| 11  | CL    | 124    |                  |
| 12  | AM    | 118    |                  |
| 12  | CM    | 118    |                  |
| 13  | AN    | 101    |                  |
| 13  | CN    | 101    |                  |
| 14  | AO    | 89     |                  |
| 14  | CO    | 89     |                  |
| 15  | AP    | 82     |                  |
| 15  | CP    | 82     |                  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 16  | AQ    | 84     |                  |
| 16  | CQ    | 84     |                  |
| 17  | AR    | 75     |                  |
| 17  | CR    | 75     |                  |
| 18  | AS    | 92     |                  |
| 18  | CS    | 92     |                  |
| 19  | AT    | 87     |                  |
| 19  | CT    | 87     |                  |
| 20  | AB    | 241    |                  |
| 20  | CB    | 241    |                  |
| 21  | AU    | 71     |                  |
| 21  | CU    | 71     |                  |
| 22  | BA    | 120    |                  |
| 22  | DA    | 120    |                  |
| 23  | BB    | 2904   |                  |
| 23  | DB    | 2904   |                  |
| 24  | BV    | 94     |                  |
| 24  | DV    | 94     |                  |
| 25  | BC    | 273    |                  |
| 25  | DC    | 273    |                  |
| 26  | BD    | 209    |                  |
| 26  | DD    | 209    |                  |
| 27  | BE    | 201    |                  |
| 27  | DE    | 201    |                  |
| 28  | BF    | 179    |                  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 28  | DF    | 179    |                  |
| 29  | BG    | 177    |                  |
| 29  | DG    | 177    |                  |
| 30  | BH    | 149    |                  |
| 30  | DH    | 149    |                  |
| 31  | BJ    | 142    |                  |
| 31  | DJ    | 142    |                  |
| 32  | BK    | 123    |                  |
| 32  | DK    | 123    |                  |
| 33  | BL    | 144    |                  |
| 33  | DL    | 144    |                  |
| 34  | BM    | 136    |                  |
| 34  | DM    | 136    |                  |
| 35  | BN    | 127    |                  |
| 35  | DN    | 127    |                  |
| 36  | BO    | 117    |                  |
| 36  | DO    | 117    |                  |
| 37  | BP    | 115    |                  |
| 37  | DP    | 115    |                  |
| 38  | BQ    | 118    |                  |
| 38  | DQ    | 118    |                  |
| 39  | BR    | 103    |                  |
| 39  | DR    | 103    |                  |
| 40  | BS    | 110    |                  |
| 40  | DS    | 110    |                  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 41  | BT    | 100    |                  |
| 41  | DT    | 100    |                  |
| 42  | BU    | 104    |                  |
| 42  | DU    | 104    |                  |
| 43  | BW    | 85     |                  |
| 43  | DW    | 85     |                  |
| 44  | BX    | 63     |                  |
| 44  | DX    | 63     |                  |
| 45  | BY    | 59     |                  |
| 45  | DY    | 59     |                  |
| 46  | BZ    | 70     |                  |
| 46  | DZ    | 70     |                  |
| 47  | B0    | 57     |                  |
| 47  | D0    | 57     |                  |
| 48  | B1    | 55     |                  |
| 48  | D1    | 55     |                  |
| 49  | B2    | 46     |                  |
| 49  | D2    | 46     |                  |
| 50  | B3    | 65     |                  |
| 50  | D3    | 65     |                  |
| 51  | B4    | 38     |                  |
| 51  | D4    | 38     |                  |
| 52  | BI    | 142    |                  |
| 52  | DI    | 142    |                  |

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 crite-

ria:

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 54  | MG   | DB    | 3093 | -         | -        | -       | X                |

## 2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 284160 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1   | AA    | 1530     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32831 | 14642 | 6024 | 10635 | 1530 |         |         |       |
| 1   | CA    | 1530     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32831 | 14642 | 6024 | 10635 | 1530 |         |         |       |

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | AC    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1624  | 1028 | 305 | 288 | 3 |         |         |       |
| 2   | CC    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1624  | 1028 | 305 | 288 | 3 |         |         |       |

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | AD    | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1643  | 1026 | 315 | 298 | 4 |         |         |       |
| 3   | CD    | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1643  | 1026 | 315 | 298 | 4 |         |         |       |

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | AE    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1105  | 687 | 211 | 201 | 6 |         |         |       |
| 4   | CE    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1105  | 687 | 211 | 201 | 6 |         |         |       |

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S6.



| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | AF    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 817   | 515 | 148 | 148 | 6 |         |         |       |
| 5   | CF    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 817   | 515 | 148 | 148 | 6 |         |         |       |

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | AG    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1174  | 730 | 226 | 214 | 4 |         |         |       |
| 6   | CG    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1196  | 745 | 230 | 217 | 4 |         |         |       |

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | AH    | 129      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 979   | 616 | 173 | 184 | 6 |         |         |       |
| 7   | CH    | 129      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 979   | 616 | 173 | 184 | 6 |         |         |       |

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | AI    | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1022  | 634 | 206 | 179 | 3 |         |         |       |
| 8   | CI    | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1022  | 634 | 206 | 179 | 3 |         |         |       |

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9   | AJ    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 786   | 493 | 150 | 142 | 1 |         |         |       |
| 9   | CJ    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 786   | 493 | 150 | 142 | 1 |         |         |       |

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | AK    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 877   | 540 | 174 | 160 | 3 |         |         |       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | CK    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 877   | 540 | 174 | 160 | 3 |         |         |       |

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | AL    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 955   | 590 | 196 | 165 | 4 |         |         |       |
| 11  | CL    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 955   | 590 | 196 | 165 | 4 |         |         |       |

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | AM    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 883   | 546 | 178 | 156 | 3 |         |         |       |
| 12  | CM    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 876   | 541 | 177 | 155 | 3 |         |         |       |

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | AN    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 774   | 483 | 160 | 128 | 3 |         |         |       |
| 13  | CN    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 774   | 483 | 160 | 128 | 3 |         |         |       |

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14  | AO    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 716   | 440 | 146 | 129 | 1 |         |         |       |
| 14  | CO    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 716   | 440 | 146 | 129 | 1 |         |         |       |

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | AP    | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 649   | 406 | 128 | 114 | 1 |         |         |       |
| 15  | CP    | 80       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 638   | 400 | 126 | 111 | 1 |         |         |       |

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | AQ    | 80       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 648   | 411 | 121 | 113 | 3 |         |         |       |
| 16  | CQ    | 81       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 657   | 417 | 122 | 115 | 3 |         |         |       |

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S18.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 17  | AR    | 55       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 455   | 288 | 86 | 81 |         |         |       |
| 17  | CR    | 55       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 455   | 288 | 86 | 81 |         |         |       |

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 18  | AS    | 79       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 637   | 408 | 120 | 107 | 2 |         |         |       |
| 18  | CS    | 80       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 644   | 413 | 121 | 108 | 2 |         |         |       |

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | AT    | 85       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 665   | 411 | 137 | 114 | 3 |         |         |       |
| 19  | CT    | 85       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 665   | 411 | 137 | 114 | 3 |         |         |       |

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 20  | AB    | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1704  | 1081 | 305 | 311 | 7 |         |         |       |
| 20  | CB    | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1704  | 1081 | 305 | 311 | 7 |         |         |       |

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S21.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 21  | AU    | 51       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 425   | 265 | 86 | 73 | 1 |         |         |       |
| 21  | CU    | 51       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 425   | 265 | 86 | 73 | 1 |         |         |       |

- Molecule 22 is a RNA chain called 5S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 22  | BA    | 117      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2507  | 1116 | 459 | 815 | 117 |         |         |       |
| 22  | DA    | 117      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2507  | 1116 | 459 | 815 | 117 |         |         |       |

- Molecule 23 is a RNA chain called 23S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 23  | BB    | 2841     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 60995 | 27210 | 11229 | 19715 | 2841 |         |         |       |
| 23  | DB    | 2841     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 60995 | 27210 | 11229 | 19715 | 2841 |         |         |       |

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24  | BV    | 94       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 753   | 479 | 137 | 134 | 3 |         |         |       |
| 24  | DV    | 94       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 753   | 479 | 137 | 134 | 3 |         |         |       |

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 25  | BC    | 267      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2053  | 1271 | 416 | 359 | 7 |         |         |       |
| 25  | DC    | 267      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2053  | 1271 | 416 | 359 | 7 |         |         |       |

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26  | BD    | 209      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1565  | 979 | 288 | 294 | 4 |         |         |       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26  | DD    | 209      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1565  | 979 | 288 | 294 | 4 |         |         |       |

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L4.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 27  | BE    | 201      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1552  | 974 | 283 | 290 | 5 |         |         |       |
| 27  | DE    | 201      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1552  | 974 | 283 | 290 | 5 |         |         |       |

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28  | BF    | 178      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1420  | 905 | 251 | 258 | 6 |         |         |       |
| 28  | DF    | 178      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1420  | 905 | 251 | 258 | 6 |         |         |       |

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29  | BG    | 176      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1323  | 832 | 243 | 246 | 2 |         |         |       |
| 29  | DG    | 176      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1323  | 832 | 243 | 246 | 2 |         |         |       |

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30  | BH    | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1111  | 699 | 197 | 214 | 1 |         |         |       |
| 30  | DH    | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1111  | 699 | 197 | 214 | 1 |         |         |       |

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31  | BJ    | 140      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1112  | 704 | 210 | 194 | 4 |         |         |       |
| 31  | DJ    | 140      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1112  | 704 | 210 | 194 | 4 |         |         |       |

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32  | BK    | 121      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 930   | 582 | 179 | 164 | 5 |         |         |       |
| 32  | DK    | 121      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 930   | 582 | 179 | 164 | 5 |         |         |       |

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33  | BL    | 144      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1053  | 654 | 207 | 190 | 2 |         |         |       |
| 33  | DL    | 144      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1053  | 654 | 207 | 190 | 2 |         |         |       |

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34  | BM    | 136      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1074  | 686 | 205 | 177 | 6 |         |         |       |
| 34  | DM    | 136      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1074  | 686 | 205 | 177 | 6 |         |         |       |

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35  | BN    | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1008  | 621 | 204 | 178 | 5 |         |         |       |
| 35  | DN    | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1008  | 621 | 204 | 178 | 5 |         |         |       |

- Molecule 36 is a protein called 50S RIBOSOMAL PROTEIN L18.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36  | BO    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 900   | 557 | 179 | 163 | 1 |         |         |       |
| 36  | DO    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 900   | 557 | 179 | 163 | 1 |         |         |       |

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37  | BP    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |         |       |
| 37  | DP    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |         |       |

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38  | BQ    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |   |         |         |       |
| 38  | DQ    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |   |         |         |       |

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39  | BR    | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |         |       |
| 39  | DR    | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |         |       |

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40  | BS    | 110      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |         |       |
| 40  | DS    | 110      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |         |       |

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41  | BT    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 777   | 491 | 145 | 139 | 2 |         |         |       |
| 41  | DT    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 777   | 491 | 145 | 139 | 2 |         |         |       |

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | BU    | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 779   | 492 | 146 | 141 |   |         |         |       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 42  | DU    | 102      | Total | C   | N   | O   |         |         |       |
|     |       |          | 779   | 492 | 146 | 141 | 0       | 0       | 0     |

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43  | BW    | 84       | Total | C   | N   | O   | S |         |         |       |
|     |       |          | 634   | 391 | 129 | 113 | 1 | 0       | 0       | 0     |
| 43  | DW    | 84       | Total | C   | N   | O   | S |         |         |       |
|     |       |          | 634   | 391 | 129 | 113 | 1 | 0       | 0       | 0     |

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L29.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 44  | BX    | 63       | Total | C   | N  | O  | S |         |         |       |
|     |       |          | 509   | 313 | 99 | 95 | 2 | 0       | 0       | 0     |
| 44  | DX    | 63       | Total | C   | N  | O  | S |         |         |       |
|     |       |          | 509   | 313 | 99 | 95 | 2 | 0       | 0       | 0     |

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L30.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 45  | BY    | 58       | Total | C   | N  | O  | S |         |         |       |
|     |       |          | 449   | 281 | 87 | 79 | 2 | 0       | 0       | 0     |
| 45  | DY    | 58       | Total | C   | N  | O  | S |         |         |       |
|     |       |          | 449   | 281 | 87 | 79 | 2 | 0       | 0       | 0     |

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L31.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46  | BZ    | 70       | Total | C   | N   | O   | S |         |         |       |
|     |       |          | 549   | 339 | 104 | 100 | 6 | 0       | 0       | 0     |
| 46  | DZ    | 70       | Total | C   | N   | O   | S |         |         |       |
|     |       |          | 549   | 339 | 104 | 100 | 6 | 0       | 0       | 0     |

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 47  | B0    | 56       | Total | C   | N  | O  | S |         |         |       |
|     |       |          | 444   | 269 | 94 | 80 | 1 | 0       | 0       | 0     |
| 47  | D0    | 56       | Total | C   | N  | O  | S |         |         |       |
|     |       |          | 444   | 269 | 94 | 80 | 1 | 0       | 0       | 0     |



- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L33.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 48  | B1    | 54       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 441   | 284 | 81 | 76 |         |         |       |
| 48  | D1    | 54       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 441   | 284 | 81 | 76 |         |         |       |

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 49  | B2    | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |         |       |
| 49  | D2    | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |         |       |

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 50  | B3    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |         |       |
| 50  | D3    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |         |       |

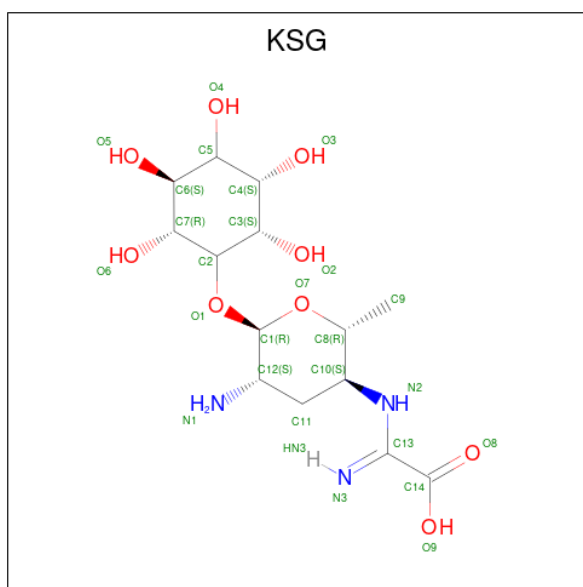
- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 51  | B4    | 38       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |         |       |
| 51  | D4    | 38       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |         |       |

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 52  | BI    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1032  | 651 | 179 | 196 | 6 |         |         |       |
| 52  | DI    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1032  | 651 | 179 | 196 | 6 |         |         |       |

- Molecule 53 is (1S,2R,3S,4R,5S,6S)-2,3,4,5,6-PENTAHYDROXYCYCLOHEXYL 2-AMINO-4-{{[CARBOXY(IMINO)METHYL]AMINO}}-2,3,4,6-TETRADEOXY-ALPHA-D-ARABINO-HEXOPYRANOSIDE (CCD ID: KSG) (formula: C<sub>14</sub>H<sub>25</sub>N<sub>3</sub>O<sub>9</sub>).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 53  | AA    | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 26    | 14 | 3 | 9 |         |         |
| 53  | CA    | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 26    | 14 | 3 | 9 |         |         |

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 54  | AA    | 60       | Total | Mg  | 0       | 0       |
|     |       |          | 60    | 60  |         |         |
| 54  | BB    | 110      | Total | Mg  | 0       | 0       |
|     |       |          | 110   | 110 |         |         |
| 54  | CA    | 62       | Total | Mg  | 0       | 0       |
|     |       |          | 62    | 62  |         |         |
| 54  | DB    | 109      | Total | Mg  | 0       | 0       |
|     |       |          | 109   | 109 |         |         |
| 54  | DE    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 54  | DN    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |

- Molecule 55 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 55  | AA    | 289      | Total | O   | 0       | 0       |
|     |       |          | 289   | 289 |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 55  | AE    | 3        | Total O<br>3 3     | 0       | 0       |
| 55  | AK    | 2        | Total O<br>2 2     | 0       | 0       |
| 55  | AN    | 3        | Total O<br>3 3     | 0       | 0       |
| 55  | AP    | 2        | Total O<br>2 2     | 0       | 0       |
| 55  | AT    | 1        | Total O<br>1 1     | 0       | 0       |
| 55  | BB    | 497      | Total O<br>497 497 | 0       | 0       |
| 55  | BC    | 1        | Total O<br>1 1     | 0       | 0       |
| 55  | BE    | 5        | Total O<br>5 5     | 0       | 0       |
| 55  | BH    | 1        | Total O<br>1 1     | 0       | 0       |
| 55  | BL    | 2        | Total O<br>2 2     | 0       | 0       |
| 55  | BN    | 1        | Total O<br>1 1     | 0       | 0       |
| 55  | CA    | 293      | Total O<br>293 293 | 0       | 0       |
| 55  | CE    | 3        | Total O<br>3 3     | 0       | 0       |
| 55  | CK    | 1        | Total O<br>1 1     | 0       | 0       |
| 55  | CL    | 4        | Total O<br>4 4     | 0       | 0       |
| 55  | CN    | 3        | Total O<br>3 3     | 0       | 0       |
| 55  | CP    | 1        | Total O<br>1 1     | 0       | 0       |
| 55  | CT    | 3        | Total O<br>3 3     | 0       | 0       |
| 55  | DB    | 501      | Total O<br>501 501 | 0       | 0       |
| 55  | DC    | 1        | Total O<br>1 1     | 0       | 0       |
| 55  | DD    | 1        | Total O<br>1 1     | 0       | 0       |

*Continued on next page...*

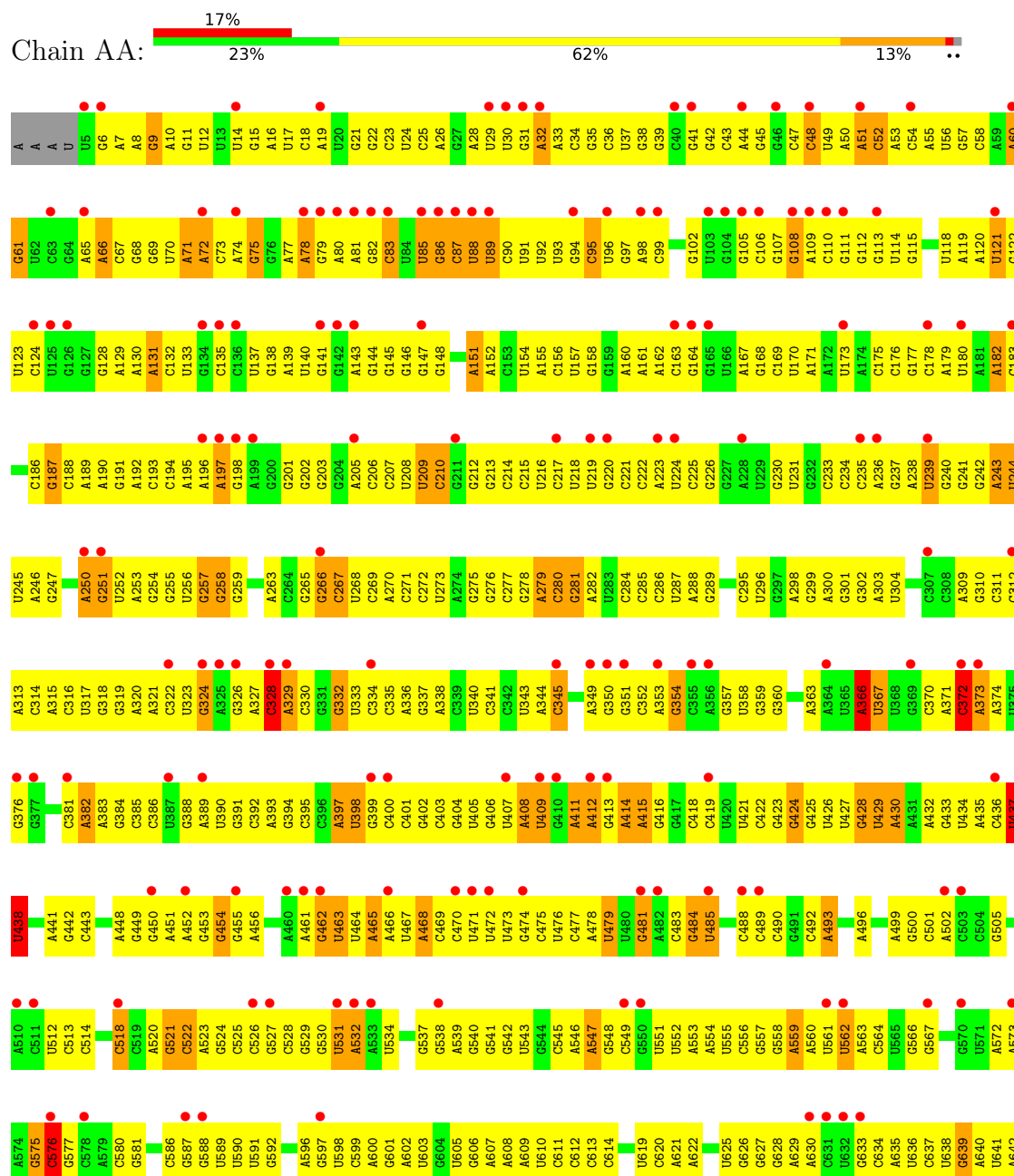
*Continued from previous page...*

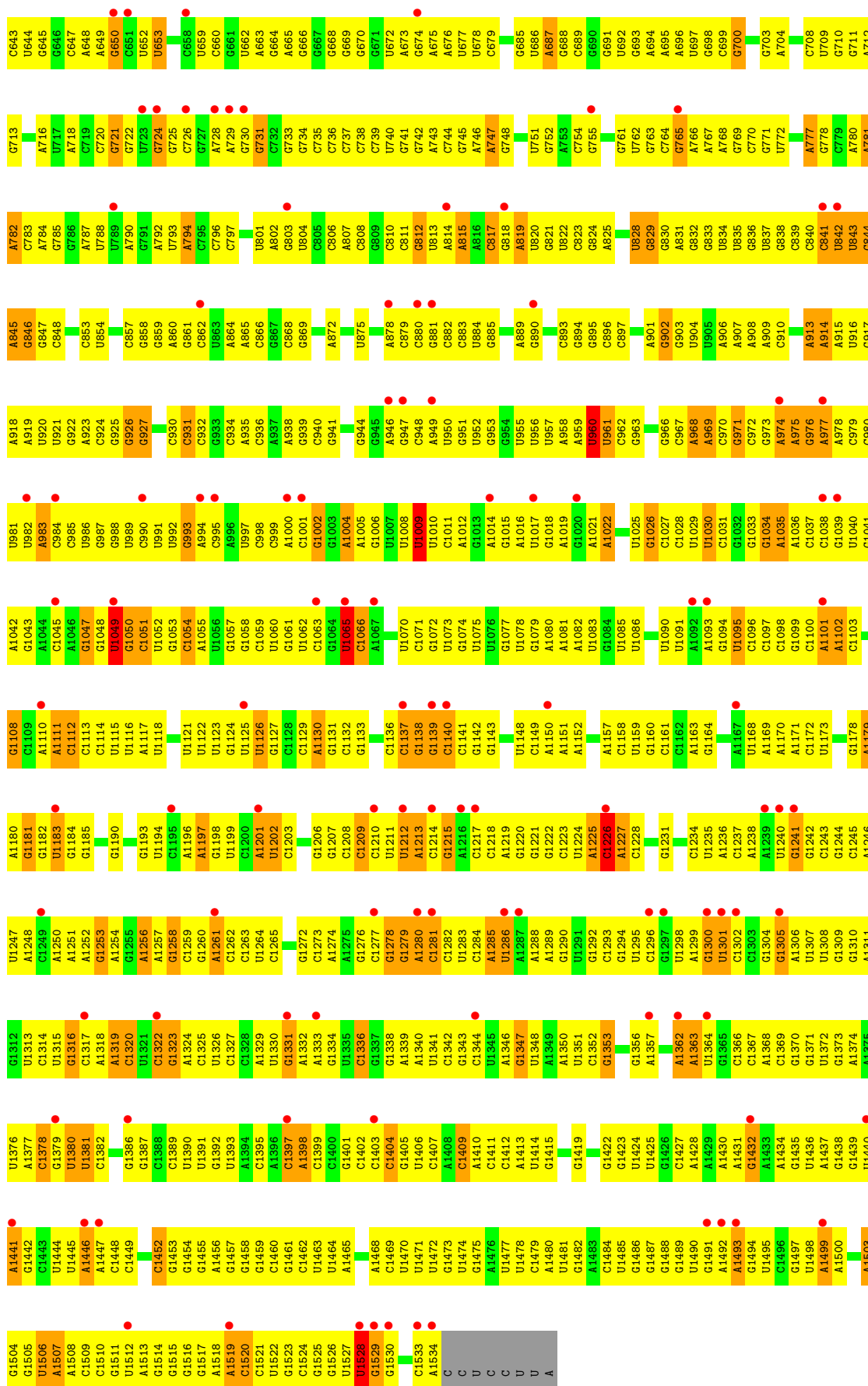
| Mol | Chain | Residues | Atoms      |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 55  | DE    | 3        | Total<br>3 | O<br>3 | 0       | 0       |
| 55  | DL    | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 55  | DN    | 2        | Total<br>2 | O<br>2 | 0       | 0       |
| 55  | DT    | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 55  | D2    | 2        | Total<br>2 | O<br>2 | 0       | 0       |

### 3 Residue-property plots

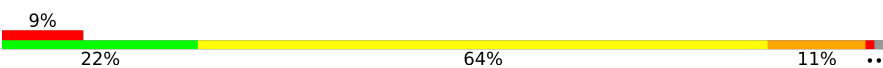
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

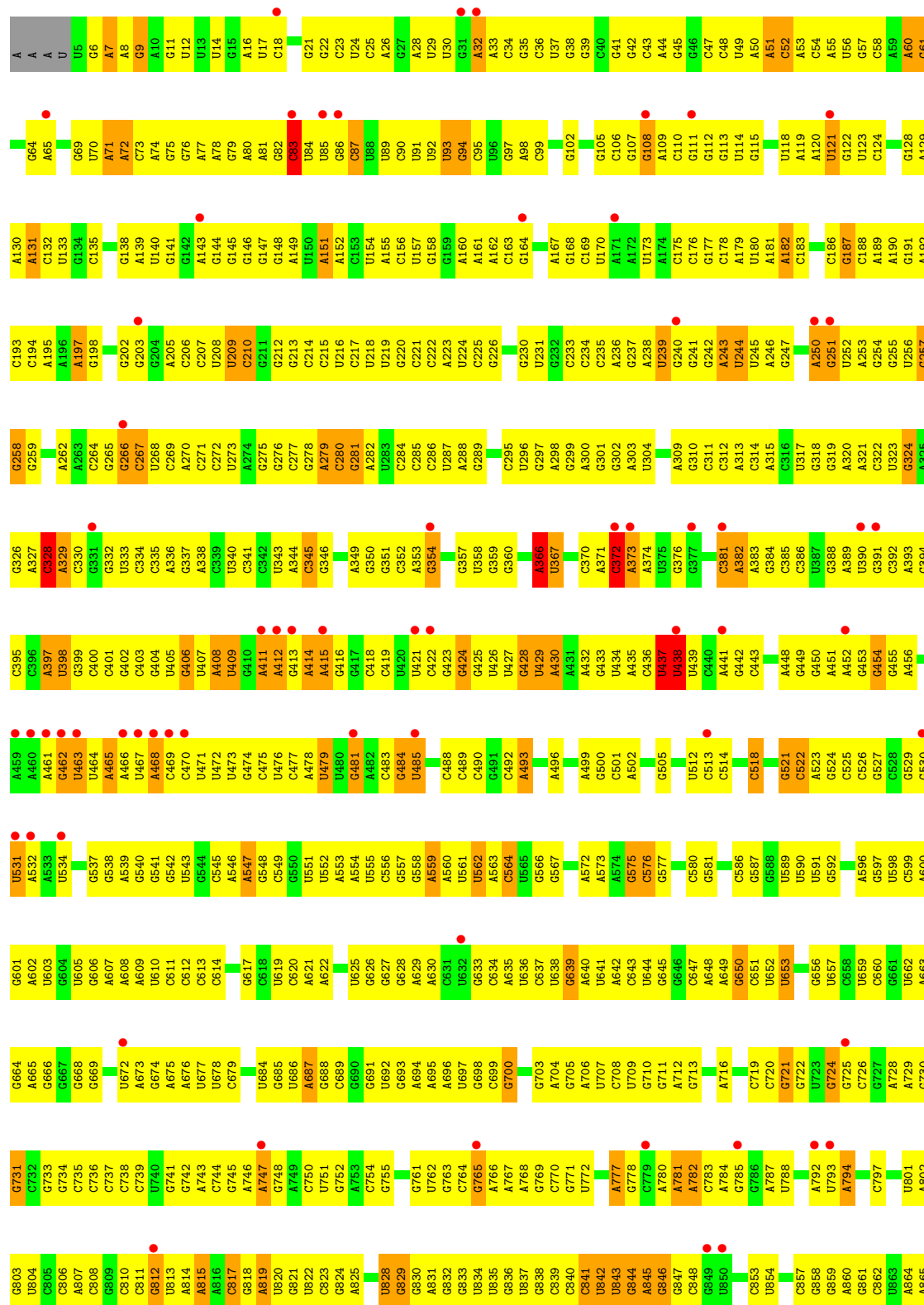
#### • Molecule 1: 16S RIBOSOMAL RNA

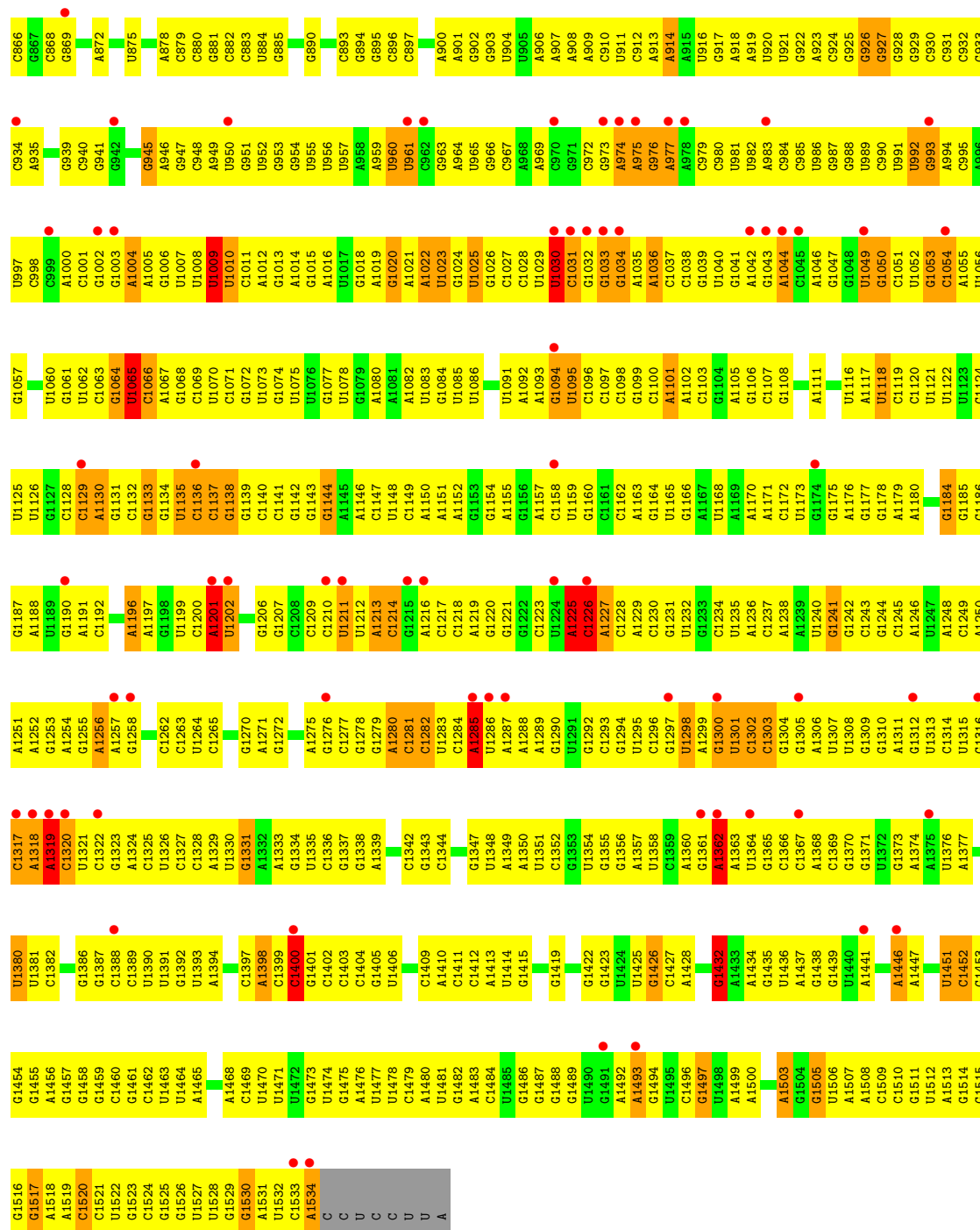




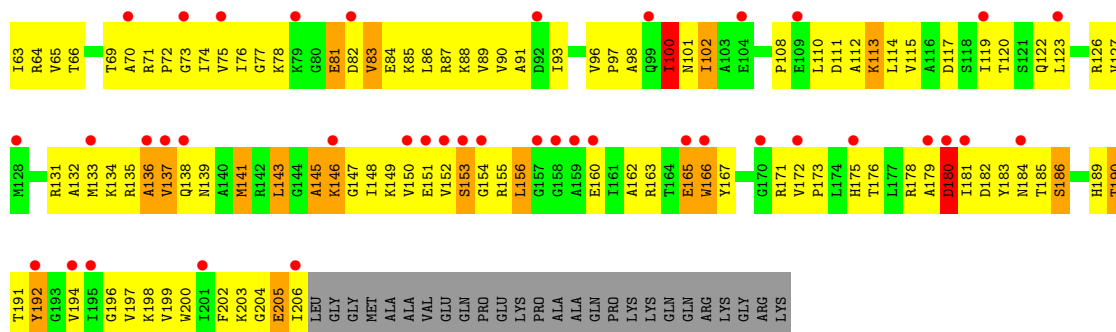
● Molecule 1: 16S RIBOSOMAL RNA

Chain CA: 

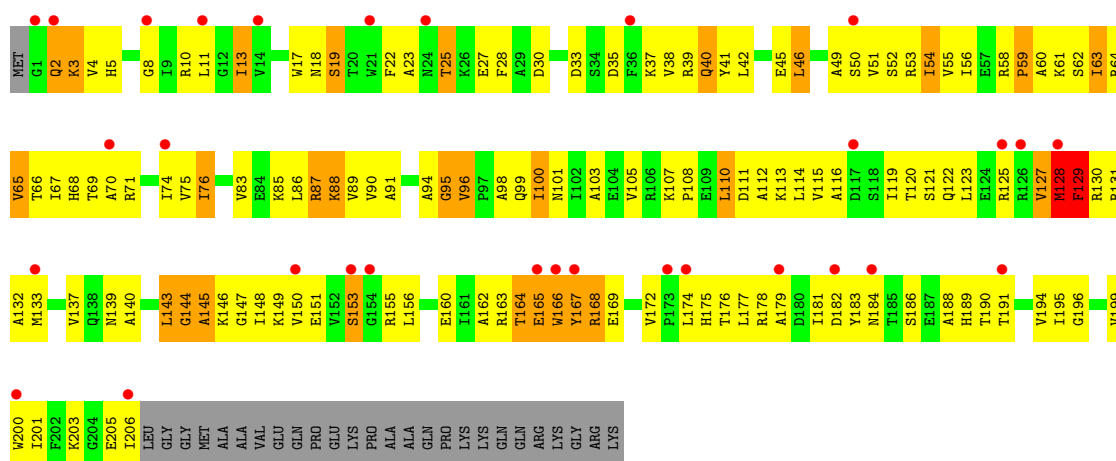




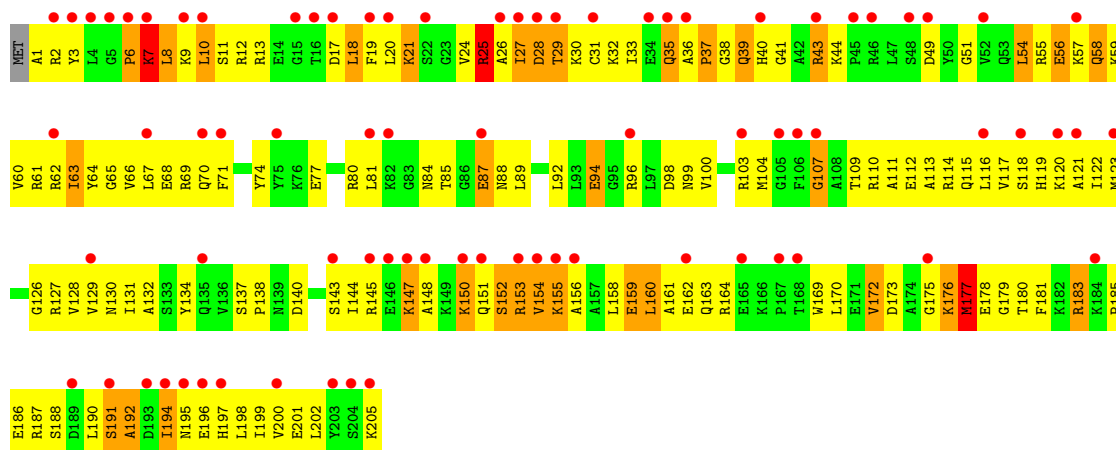




• Molecule 2: 30S RIBOSOMAL PROTEIN S3

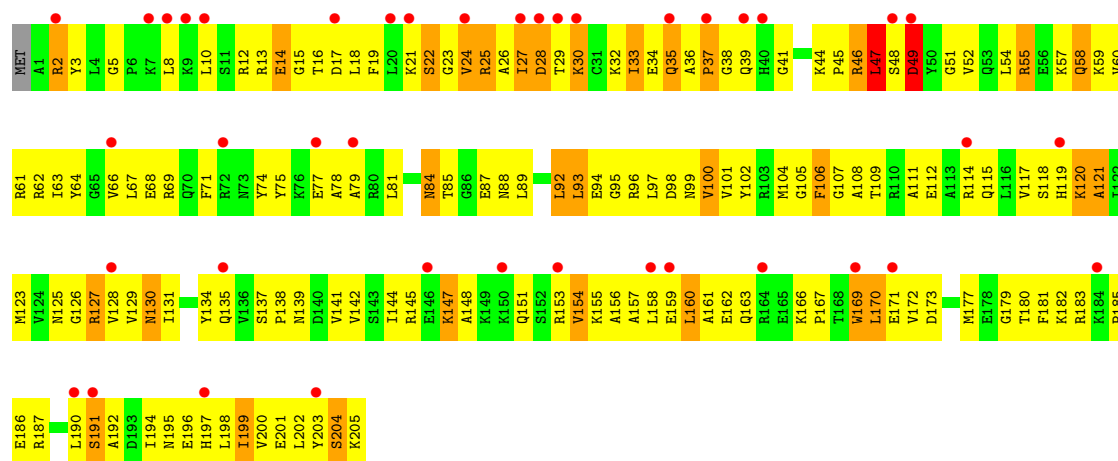


• Molecule 3: 30S RIBOSOMAL PROTEIN S4

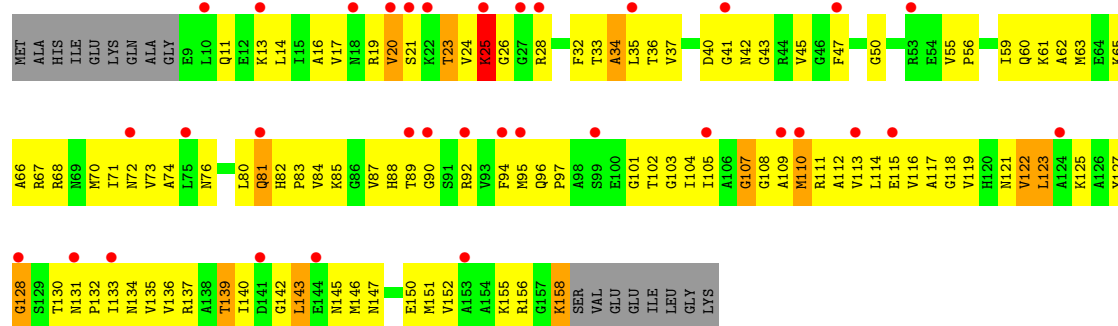


• Molecule 3: 30S RIBOSOMAL PROTEIN S4

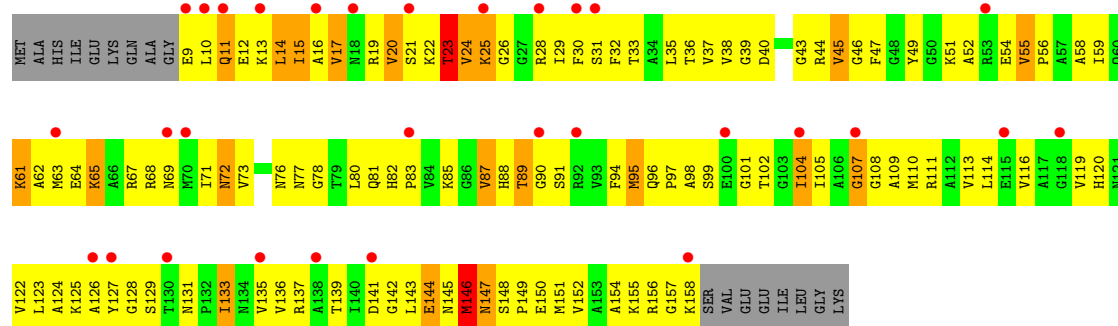




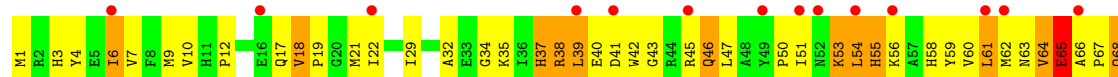
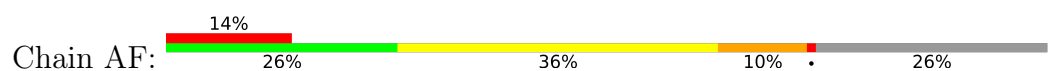
• Molecule 4: 30S RIBOSOMAL PROTEIN S5

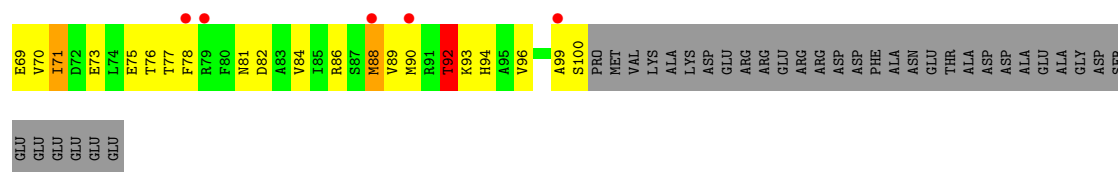


• Molecule 4: 30S RIBOSOMAL PROTEIN S5

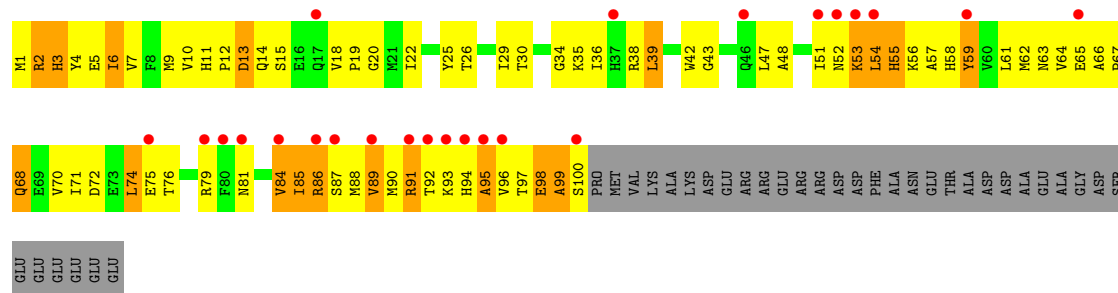
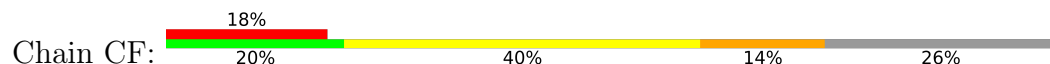


• Molecule 5: 30S RIBOSOMAL PROTEIN S6

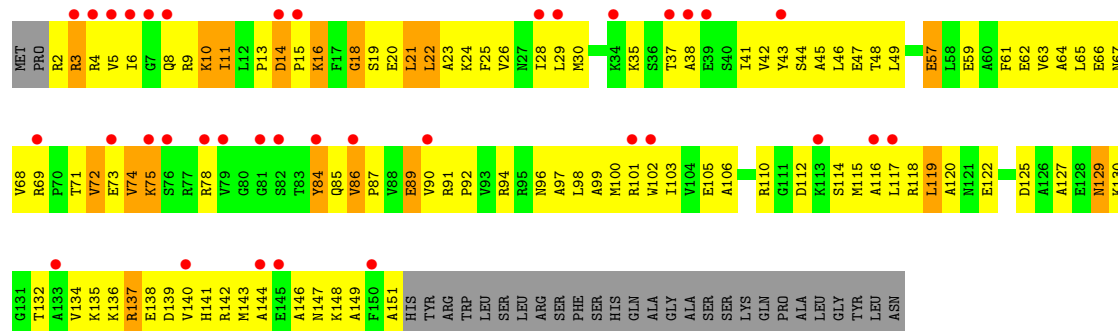




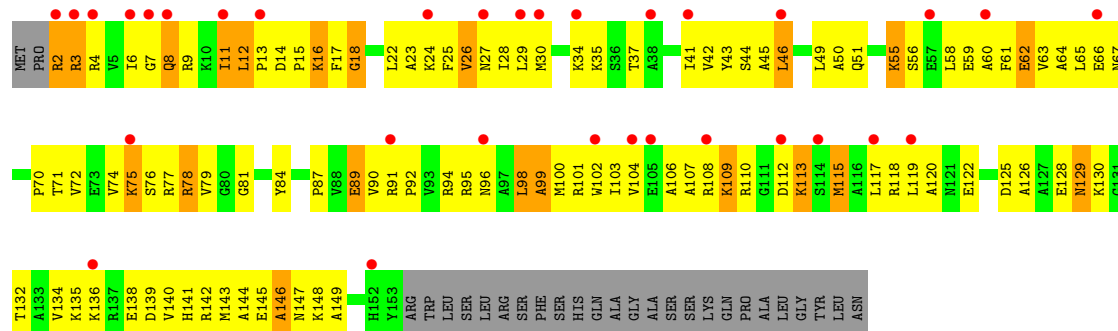
• Molecule 5: 30S RIBOSOMAL PROBLEM S6



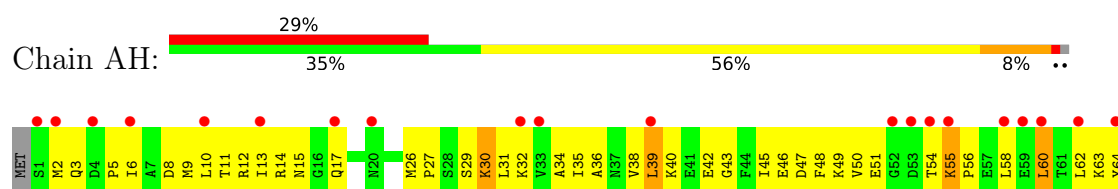
• Molecule 6: 30S RIBOSOMAL PROBLEM S7



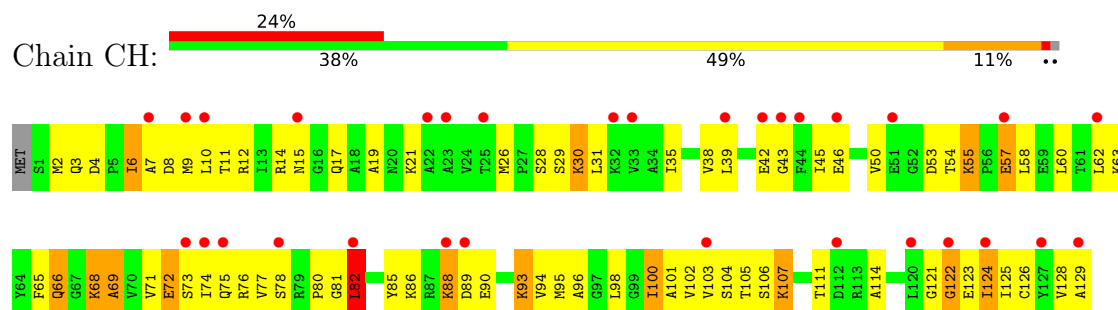
• Molecule 6: 30S RIBOSOMAL PROBLEM S7



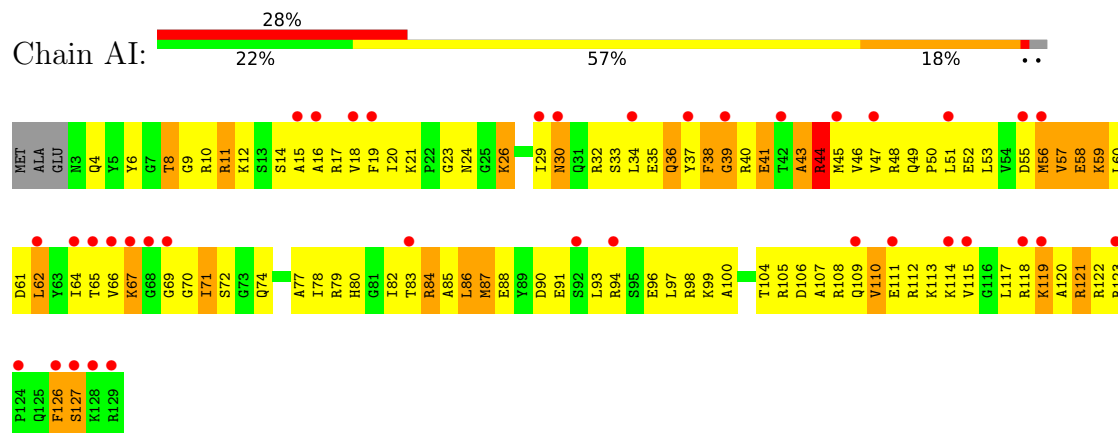
• Molecule 7: 30S RIBOSOMAL PROBLEM S8



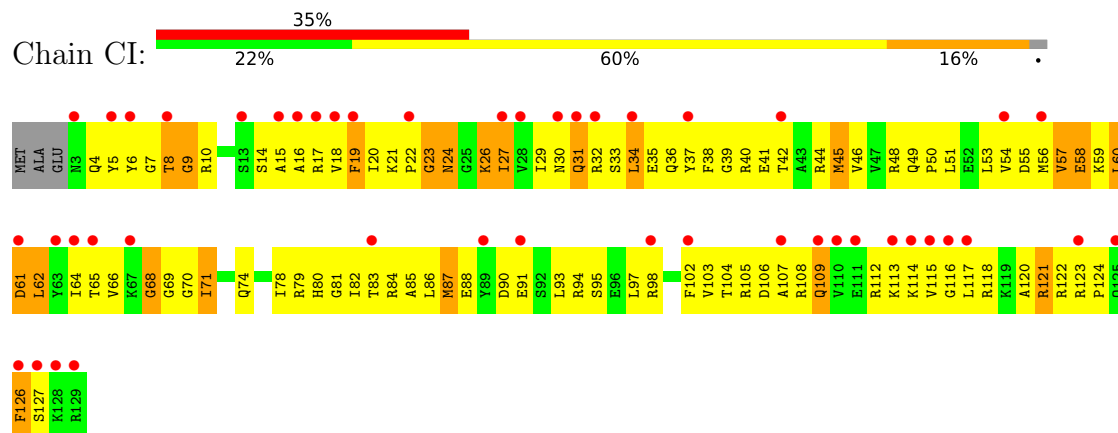
• Molecule 7: 30S RIBOSOMAL PROTEIN S8



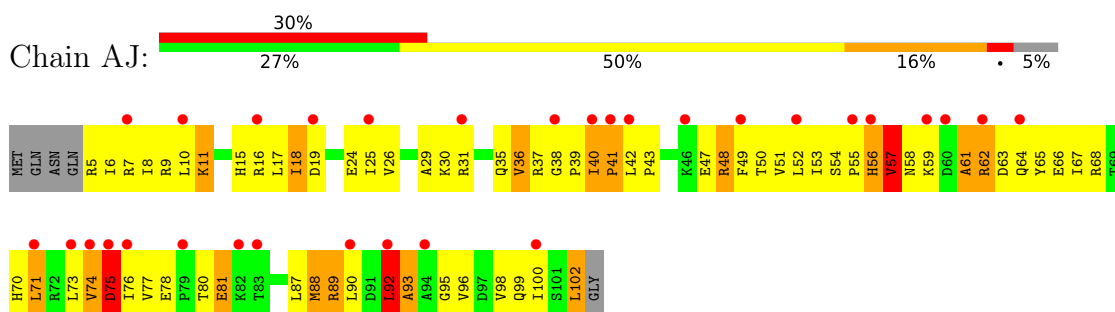
• Molecule 8: 30S RIBOSOMAL PROTEIN S9



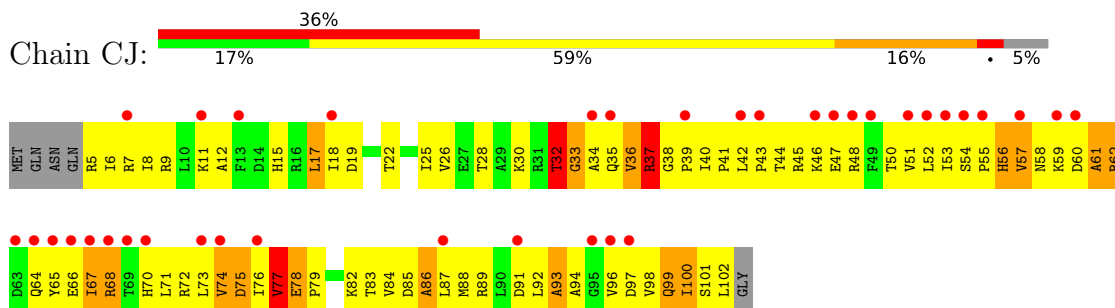
• Molecule 8: 30S RIBOSOMAL PROTEIN S9



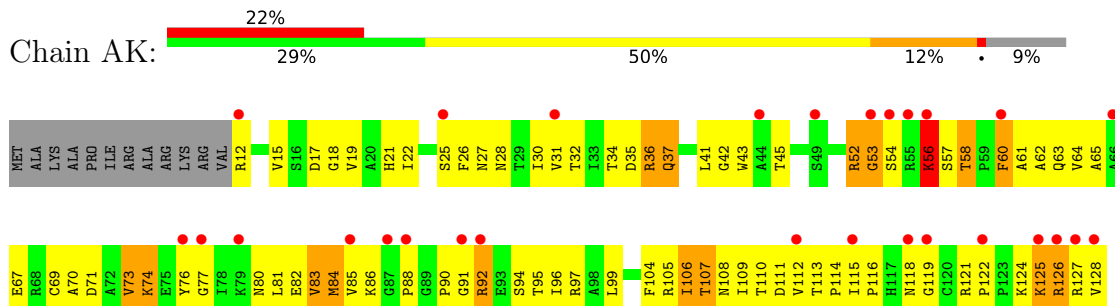
• Molecule 9: 30S RIBOSOMAL PROTEIN S10



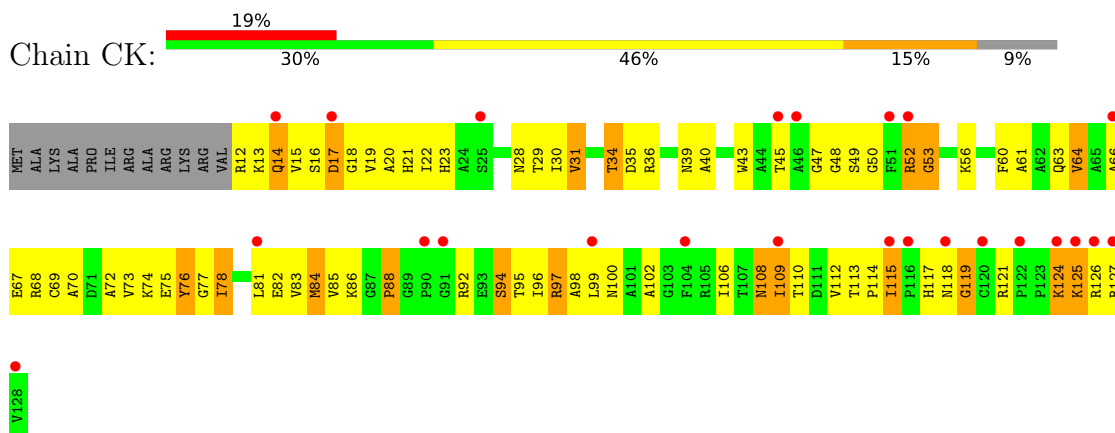
• Molecule 9: 30S RIBOSOMAL PROTEIN S10



• Molecule 10: 30S RIBOSOMAL PROTEIN S11

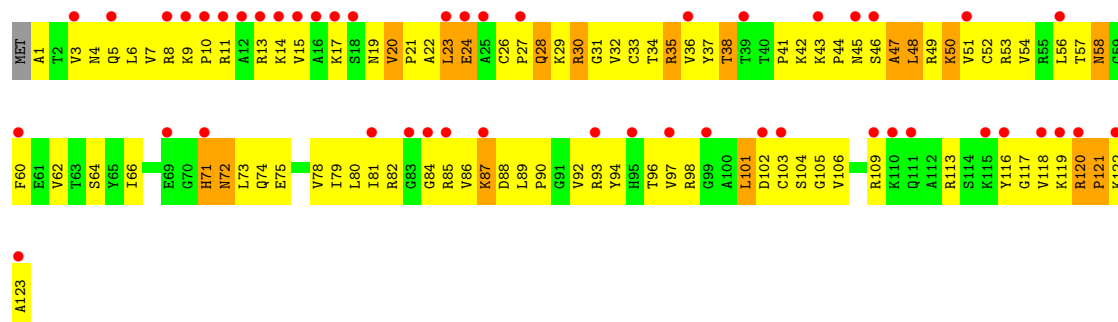


• Molecule 10: 30S RIBOSOMAL PROTEIN S11



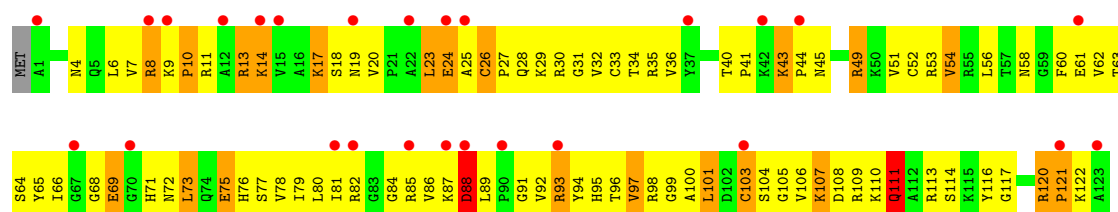
• Molecule 11: 30S RIBOSOMAL PROTEIN S12





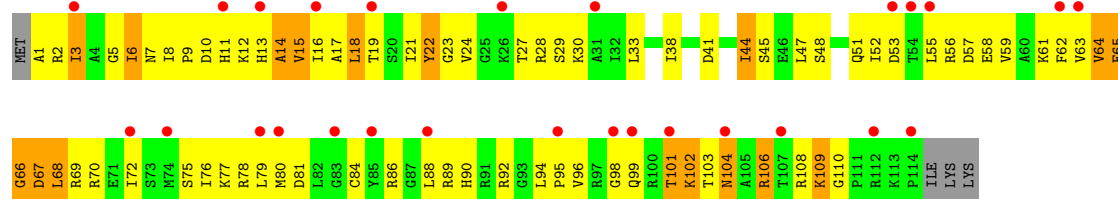
• Molecule 11: 30S RIBOSOMAL PROTEIN S12

Chain CL: 21% 25% 56% 17% ..



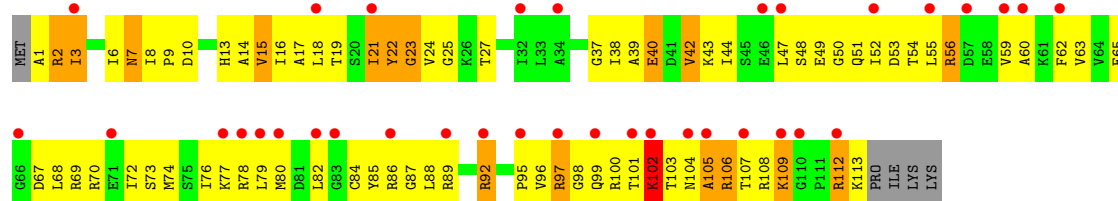
• Molecule 12: 30S RIBOSOMAL PROTEIN S13

Chain AM: 23% 31% 52% 14% .



• Molecule 12: 30S RIBOSOMAL PROTEIN S13

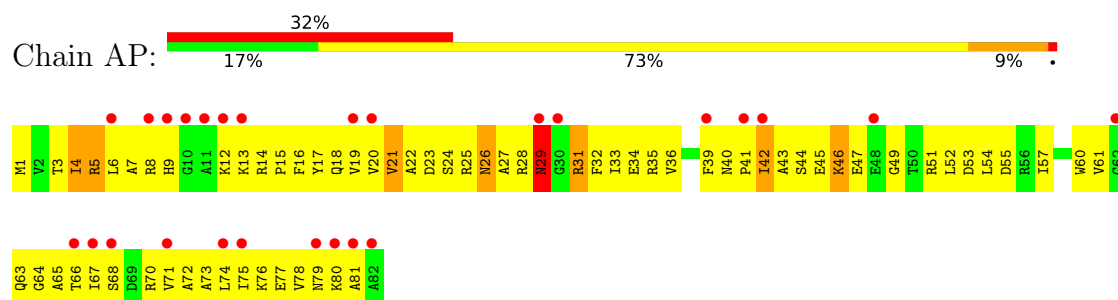
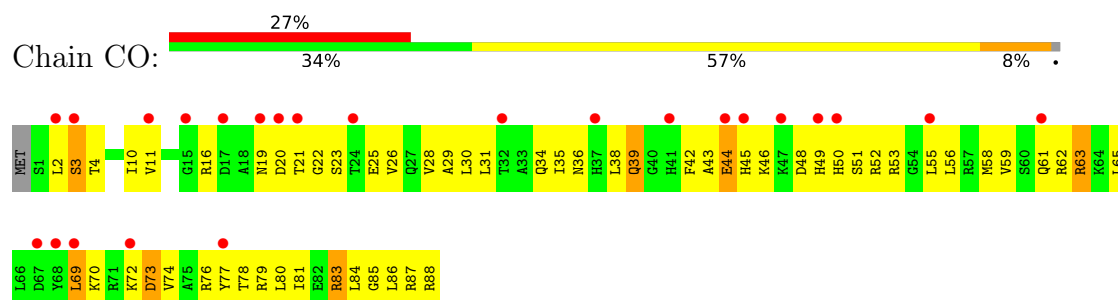
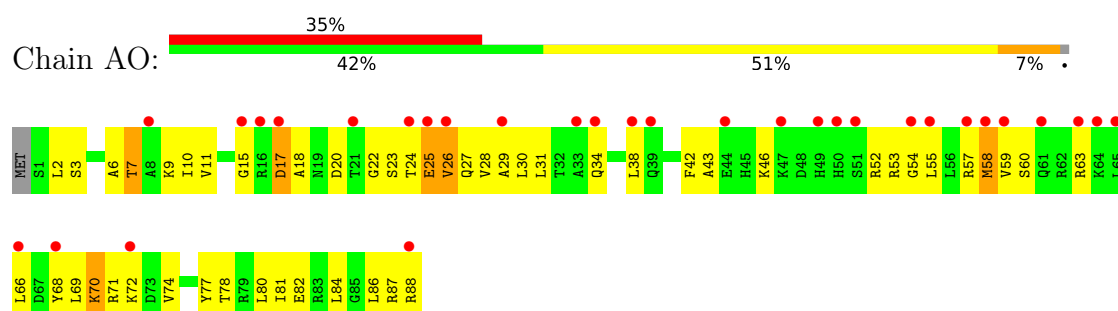
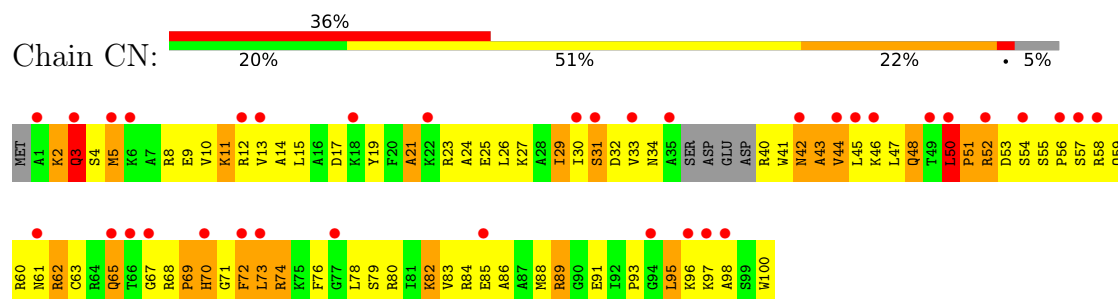
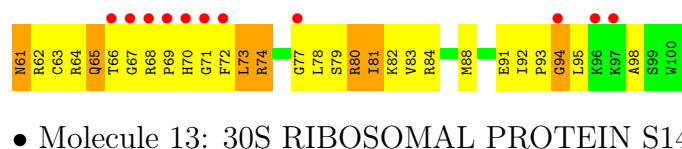
Chain CM: 30% 28% 53% 14% ..

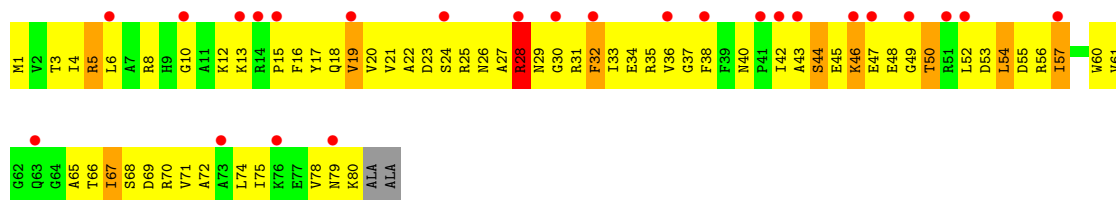


• Molecule 13: 30S RIBOSOMAL PROTEIN S14

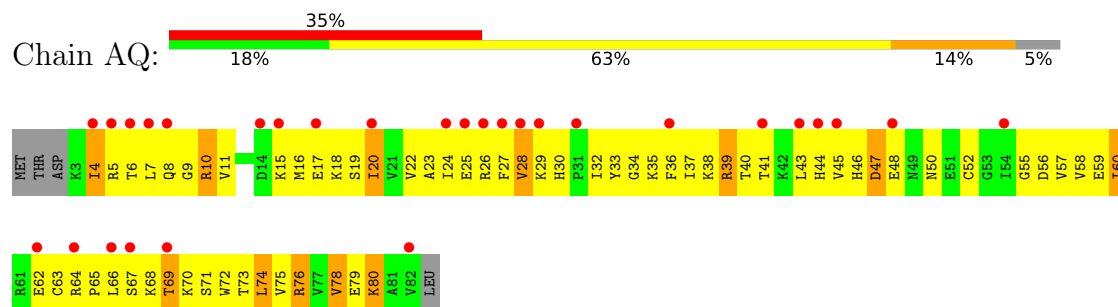
Chain AN: 43% 27% 50% 19% 5% ..



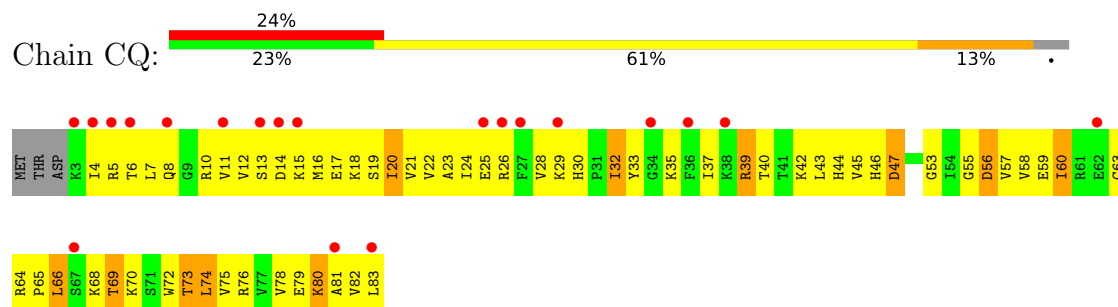




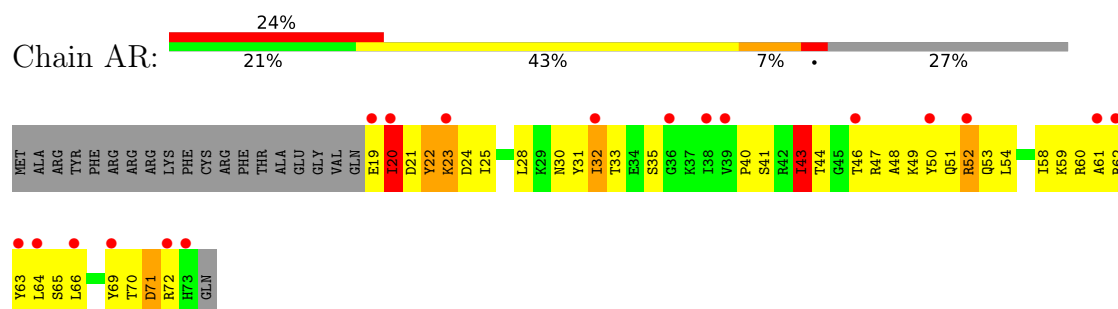
• Molecule 16: 30S RIBOSOMAL PROTEIN S17



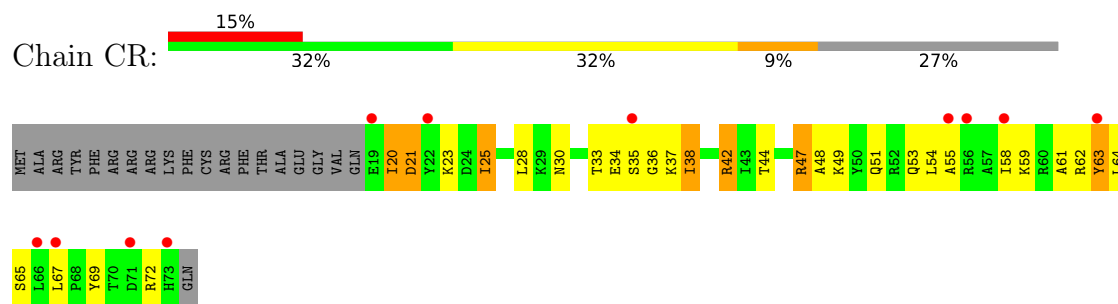
• Molecule 16: 30S RIBOSOMAL PROTEIN S17



• Molecule 17: 30S RIBOSOMAL PROTEIN S18

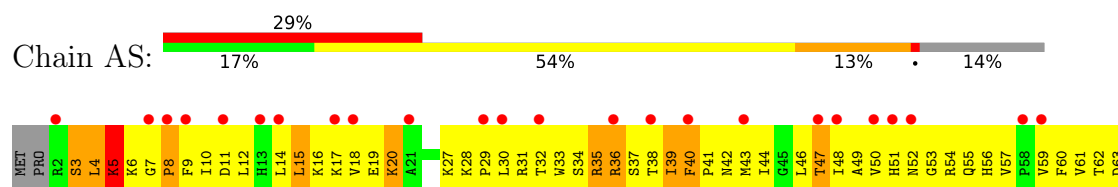


• Molecule 17: 30S RIBOSOMAL PROTEIN S18

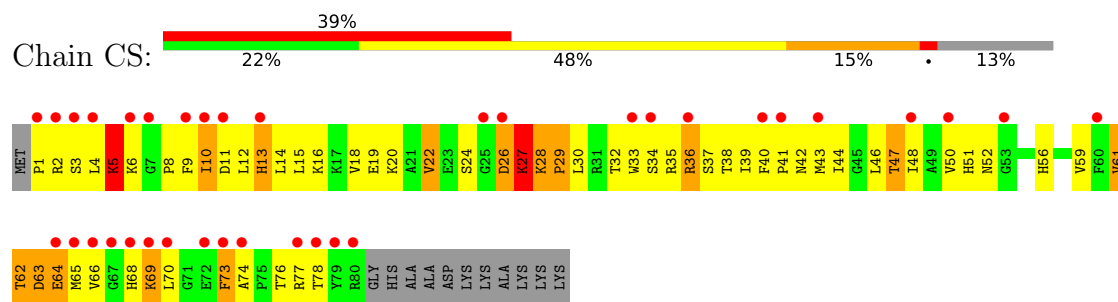


• Molecule 18: 30S RIBOSOMAL PROTEIN S19

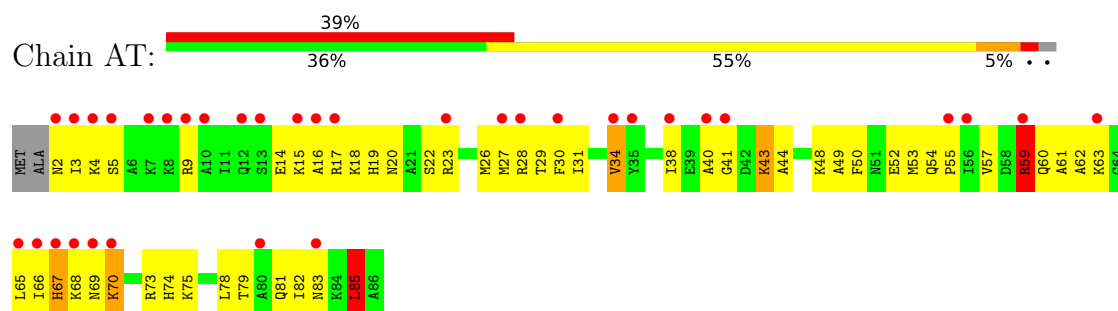




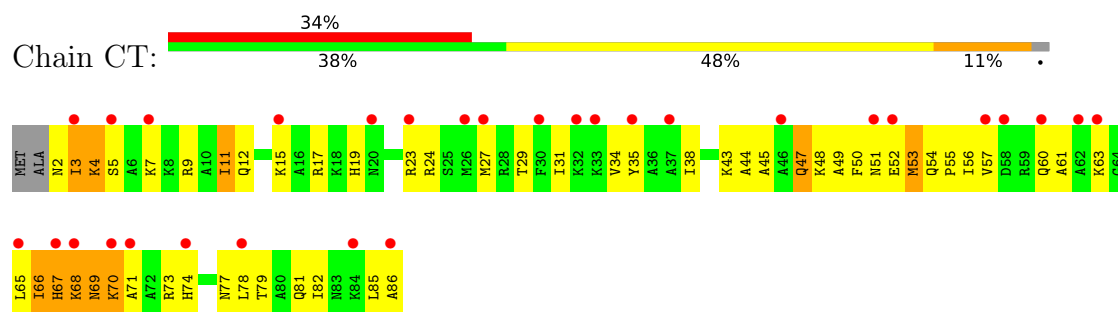
• Molecule 18: 30S RIBOSOMAL PROTEIN S19



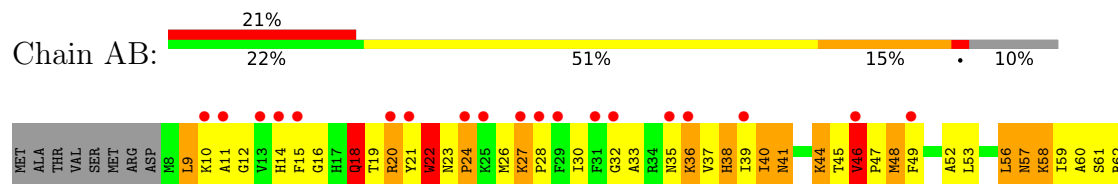
• Molecule 19: 30S RIBOSOMAL PROTEIN S20

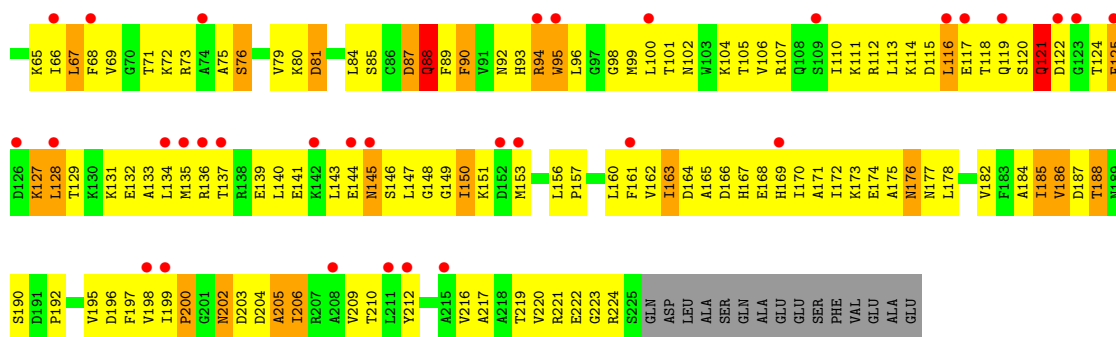


• Molecule 19: 30S RIBOSOMAL PROTEIN S20

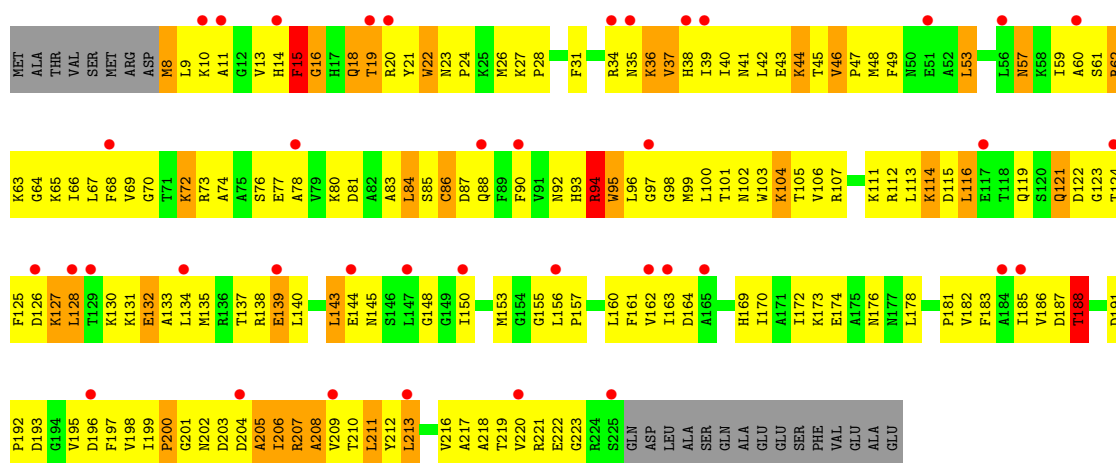


• Molecule 20: 30S RIBOSOMAL PROTEIN S2

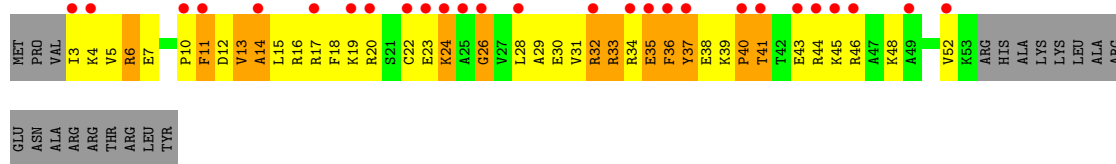




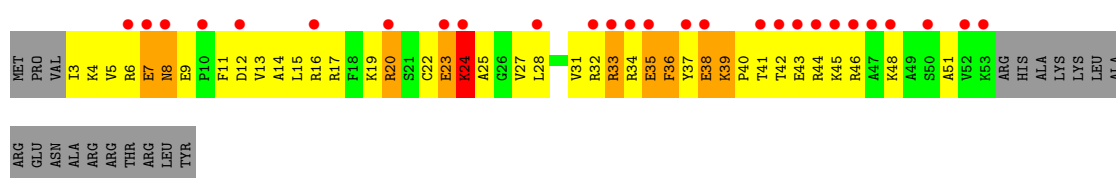
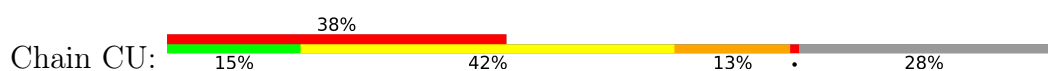
• Molecule 20: 30S RIBOSOMAL PROTEIN S2



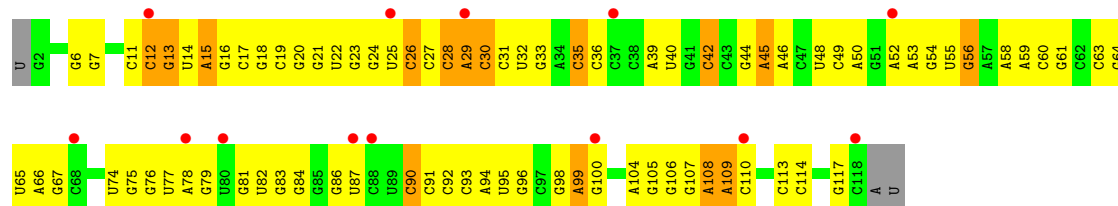
• Molecule 21: 30S RIBOSOMAL PROTEIN S21



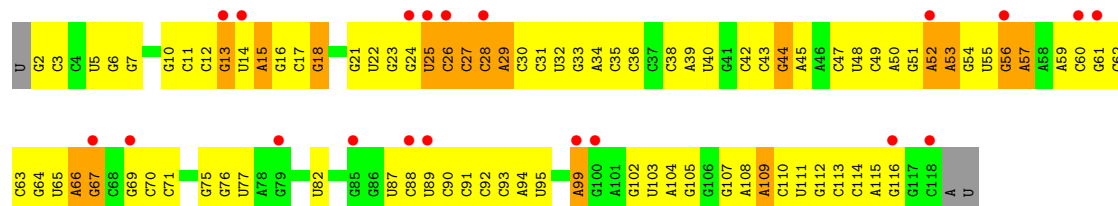
• Molecule 21: 30S RIBOSOMAL PROTEIN S21



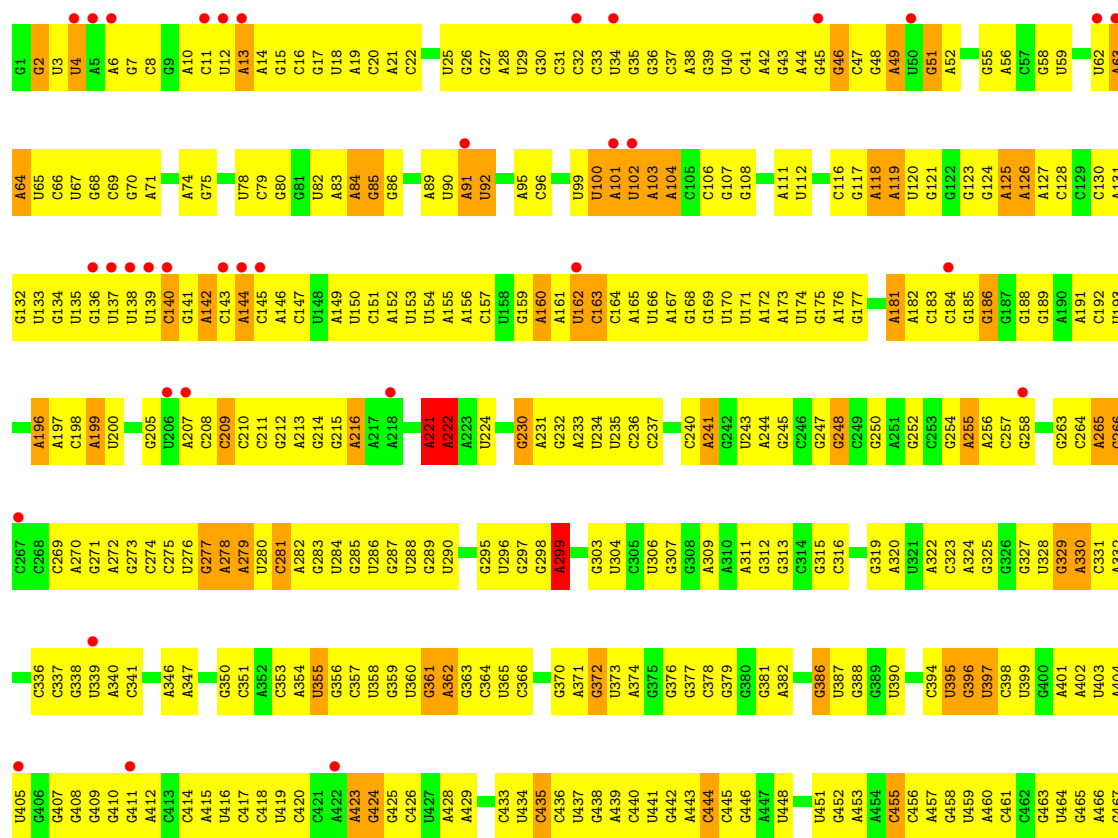
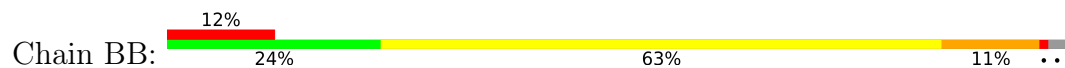
• Molecule 22: 5S RIBOSOMAL RNA

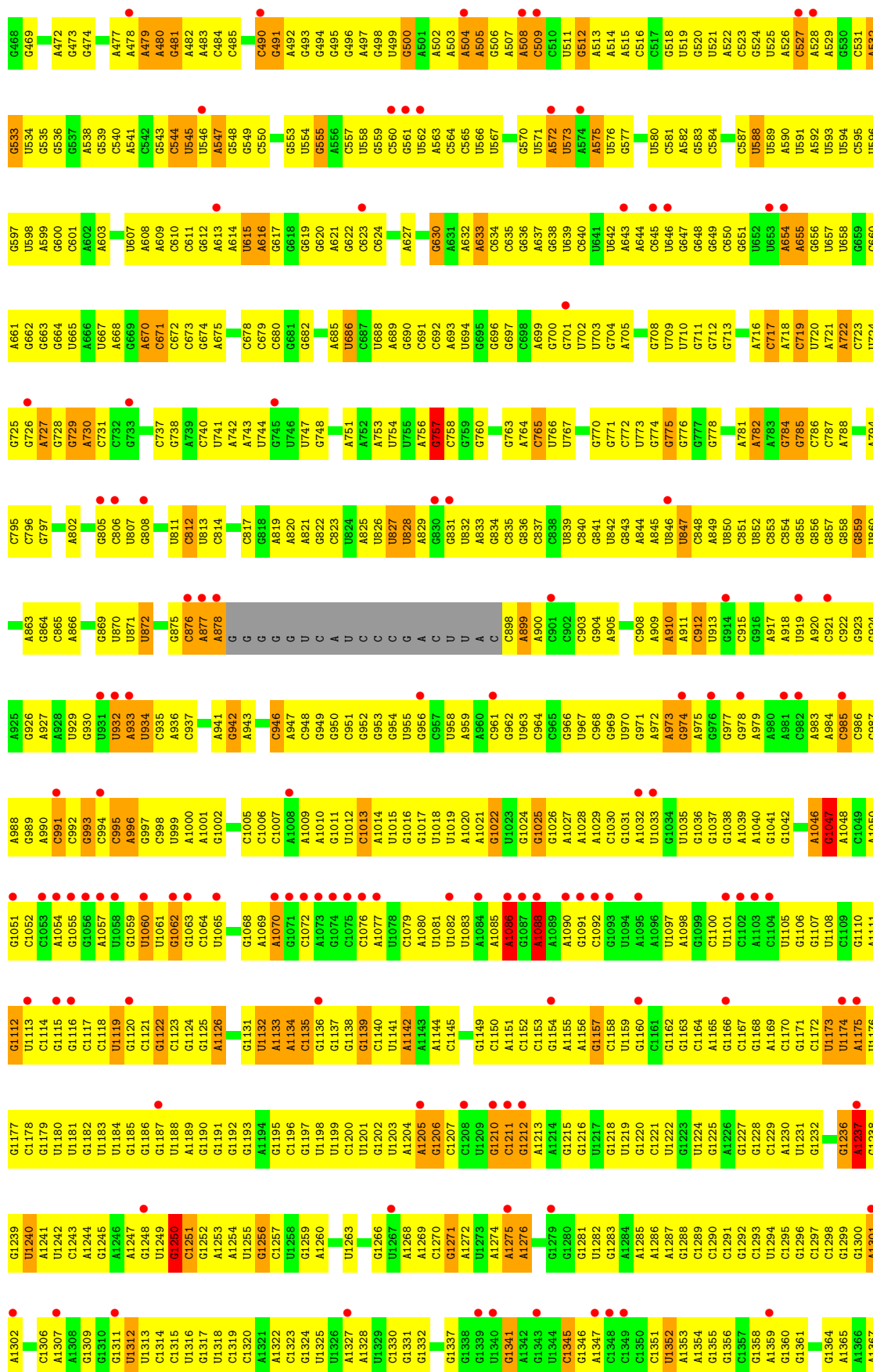


• Molecule 22: 5S RIBOSOMAL RNA

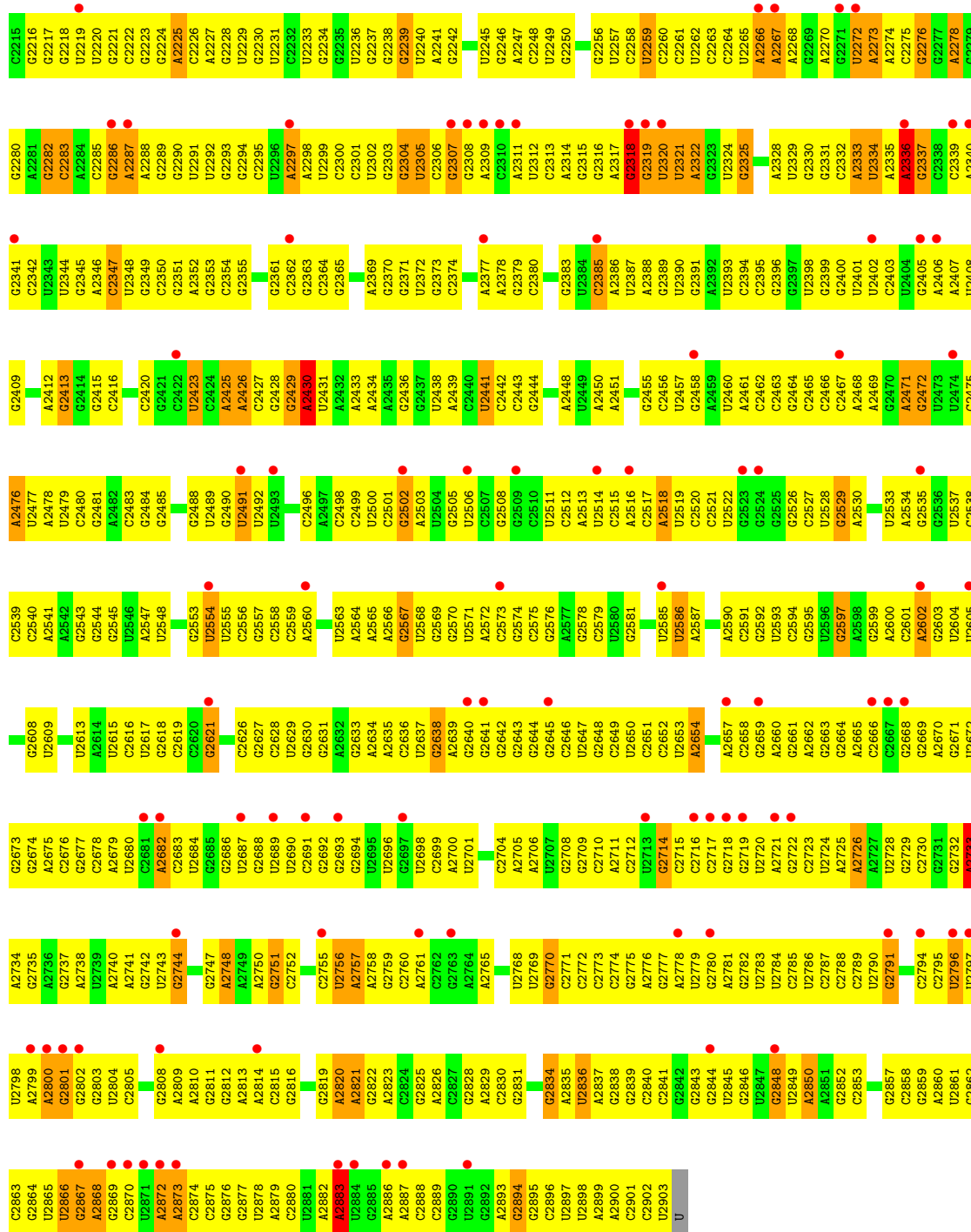


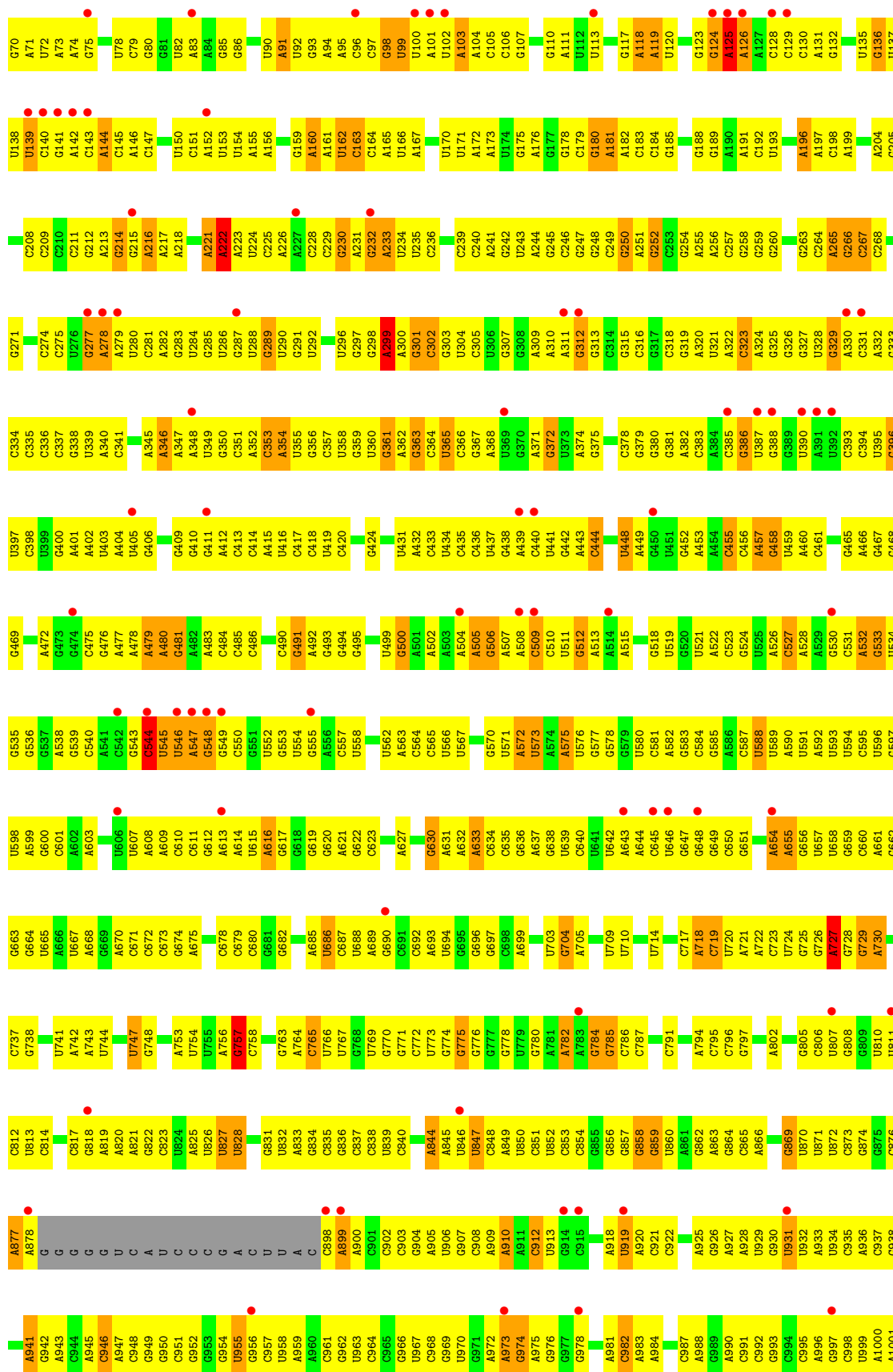
• Molecule 23: 23S RIBOSOMAL RNA





|       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| C2153 | G2093 | A2031 | G1964 | G1897 | G1824 | A1759 | G1699 | U1559 | A1494 | G1431 | G1368 |
| A2154 | A2094 | G2032 | G1965 | U1958 | U1825 | C1760 | A1634 | G1560 | A1495 | G1432 | G1369 |
| U2155 | A2095 | A2033 | A1966 | A1901 | G1826 | C1761 | U1636 | U1561 | A1496 | A1433 | G1370 |
| G2156 | C2096 | U2034 | C1967 | G1904 | U1827 | A1762 | C1637 | U1562 | U1497 | A1434 | G1371 |
| A     | A2097 | C2036 | G1970 | G1905 | G1829 | G1764 | C1638 | U1563 | C1498 | U1372 | U1372 |
| C     | U2098 | A2037 | A1971 | C1906 | A1830 | U1765 | A1640 | C1565 | C1499 | A1374 | A1373 |
| G     | U2099 | A2037 | U1971 | G1906 | C1833 | G1766 | A1641 | U1566 | U1438 | G1374 | G1374 |
| C     | G2100 | U2038 | U1972 | C1909 | C1833 | G1770 | G1642 | A1567 | A1439 | U1375 | U1375 |
| C     | A2101 | U2039 | G1973 | C1909 | C1838 | C1770 | G1645 | U1568 | U1440 | U1379 | U1379 |
| G     | G2102 | U2040 | C1974 | U1910 | C1838 | C1771 | U1646 | A1569 | G1441 | G1390 | G1390 |
| A     | C2103 | U2041 | C1974 | U1911 | A1772 | G1710 | U1647 | A1570 | U1442 | G1381 | G1381 |
| C     | G2104 | A2042 | G1975 | U1912 | A1773 | A1711 | U1648 | A1571 | U1443 | G1382 | G1382 |
| C     | U2105 | C2043 | U1976 | A1913 | C1774 | U1712 | U1649 | A1572 | G1445 | A1383 | A1383 |
| U     | U2106 | C2044 | G1976 | A1914 | C1775 | U1713 | A1650 | U1578 | C1446 | A1384 | A1384 |
| U     | G2107 | C2045 | U1979 | U1915 | U1776 | U1714 | A1651 | A1579 | C1447 | A1385 | A1385 |
| G     | A2108 | G2046 | G1980 | U1916 | U1777 | U1715 | A1652 | A1580 | G1448 | A1386 | A1386 |
| A     | U2109 | C2047 | A1981 | U1917 | U1778 | U1716 | A1653 | G1449 | U1450 | A1387 | A1387 |
| A     | A     | G2048 | G1982 | U1918 | U1779 | U1717 | G1654 | U1451 | G1450 | G1388 | G1388 |
| A     | U     | C2049 | C1985 | A1919 | A1780 | U1718 | A1654 | C1582 | C1451 | G1389 | G1389 |
| U     | G     | C2050 | C1986 | A1920 | U1781 | G1719 | A1655 | U1583 | G1452 | U1390 | U1390 |
| A     | A     | A2051 | A1987 | G1921 | U1782 | U1720 | C1656 | U1584 | A1453 | U1391 | U1391 |
| C     | C     | A2052 | G1988 | G1922 | U1783 | G1721 | U1657 | C1585 | C1454 | A1392 | A1392 |
| C     | C     | G2053 | G1989 | G1923 | A1784 | U1722 | C1658 | A1586 | G1455 | U1393 | U1393 |
| A     | A     | A2054 | C1990 | U1924 | A1785 | G1723 | G1659 | U1588 | G1456 | A1395 | A1395 |
| C     | C     | C2055 | U1991 | C1924 | A1786 | G1724 | U1661 | U1589 | U1457 | U1396 | U1396 |
| C     | U     | G2056 | G1992 | C1925 | A1787 | U1725 | U1662 | A1590 | U1458 | A1397 | A1397 |
| U     | A     | G2057 | U1993 | U1926 | C1788 | U1726 | U1663 | A1591 | C1459 | C1398 | C1398 |
| C     | G     | A2058 | A1997 | A1927 | G1862 | C1727 | U1664 | C1592 | U1460 | C1399 | C1399 |
| U     | U     | C2059 | C1998 | G1928 | U1863 | C1728 | A1664 | U1594 | C1461 | U1400 | U1400 |
| U     | G     | A2060 | C1999 | U1929 | U1864 | C1729 | A1665 | C1595 | C1462 | G1401 | G1401 |
| A     | C     | G2061 | C2000 | U1930 | U1865 | U1729 | G1666 | C1596 | C1463 | U1402 | U1402 |
| A     | G     | A2062 | C2001 | U1931 | U1866 | C1730 | G1667 | A1596 | G1464 | A1403 | A1403 |
| U     | U     | C2063 | A1992 | A1932 | A1867 | G1731 | U1668 | A1597 | G1465 | C1404 | C1404 |
| C     | A     | C2064 | G2002 | C1933 | U1795 | U1732 | A1669 | A1598 | U1466 | U1405 | U1405 |
| G     | G     | G2065 | A2003 | C1934 | G1796 | C1733 | C1670 | U1599 | U1467 | U1406 | U1406 |
| C     | C     | C2066 | G2004 | G1935 | G1797 | U1734 | U1671 | A1535 | U1468 | G1407 | G1407 |
| C     | G     | A2067 | A2005 | A1936 | U1798 | U1735 | U1672 | C1600 | A1469 | U1408 | U1408 |
| U     | U     | C2068 | C2006 | A1937 | G1799 | U1736 | G1673 | G1601 | U1470 | U1409 | U1409 |
| U     | U     | G2069 | U2007 | A1938 | C1800 | G1737 | G1674 | U1602 | G1471 | G1410 | G1410 |
| U     | U     | A2070 | C2008 | U1939 | A1801 | U1738 | C1675 | A1603 | U1474 | U1411 | U1411 |
| A     | A     | C2071 | A2009 | C1940 | A1802 | G1739 | A1676 | C1604 | G1475 | A1412 | A1412 |
| C     | C     | G2072 | C2012 | C1941 | A1803 | U1740 | C1677 | C1605 | U1476 | A1413 | A1413 |
| C     | C     | C2073 | A2013 | U1942 | A1804 | G1741 | C1678 | C1606 | U1477 | C1414 | C1414 |
| U     | U     | U2074 | A2014 | U1943 | A1805 | U1742 | A1679 | C1607 | A1478 | U1415 | U1415 |
| U     | U     | U2075 | A2015 | U1944 | A1806 | G1743 | U1680 | A1608 | G1479 | G1416 | G1416 |
| U     | U     | U2076 | A2016 | G1945 | A1807 | U1744 | U1681 | A1609 | G1479 | C1417 | C1417 |
| U     | U     | U2077 | U2016 | U1946 | A1808 | A1745 | U1682 | A1610 | C1480 | G1418 | G1418 |
| U     | U     | C2078 | U2017 | C1947 | A1809 | U1746 | U1683 | A1611 | U1481 | A1419 | A1419 |
| U     | U     | U2079 | A2019 | G1948 | A1811 | U1747 | G1684 | C1617 | C1482 | A1420 | A1420 |
| U     | U     | A2080 | A2020 | U1949 | U1812 | C1748 | C1685 | U1549 | G1483 | G1421 | G1421 |
| U     | U     | U2081 | C2021 | G1950 | G1813 | U1749 | C1686 | A1550 | U1484 | G1422 | G1422 |
| U     | U     | A2082 | U2022 | U1951 | C1816 | U1750 | U1687 | A1551 | U1485 | G1423 | G1423 |
| U     | U     | C2083 | C2023 | A1952 | A1817 | U1751 | G1688 | C1625 | U1486 | G1424 | G1424 |
| U     | U     | G2084 | G2024 | A1953 | U1818 | C1752 | U1689 | U1554 | U1487 | G1425 | G1425 |
| U     | U     | U2085 | C2025 | A1954 | A1819 | G1753 | A1690 | U1555 | C1488 | G1426 | G1426 |
| U     | U     | U2086 | U2026 | U1955 | U1820 | U1754 | A1691 | A1560 | C1489 | A1427 | A1427 |
| U     | U     | C2087 | G2027 | U1956 | U1821 | A1755 | C1691 | A1631 | U1490 | G1428 | G1428 |
| U     | U     | A2088 | U2028 | C1957 | A1822 | G1756 | U1695 | A1632 | U1491 | G1429 | G1429 |
| U     | U     | U2089 | C2029 | C1958 | A1823 | A1757 | G1696 | G1633 | C1493 | G1430 | G1430 |
| U     | U     | U2090 | A2030 | G1959 | G1823 | U1758 | U1697 | U1634 | U1494 | U1431 | U1431 |
| U     | U     | U2091 | U2091 | U1960 | U1824 | U1759 | U1698 | U1635 | U1495 | U1432 | U1432 |
| U     | U     | U2092 | U2092 | U1961 | U1825 | U1760 | U1699 | U1636 | U1496 | U1433 | U1433 |
| U     | U     | U2093 | U2093 | U1962 | U1826 | U1761 | U1700 | U1567 | U1497 | U1434 | U1434 |
| U     | U     | U2094 | U2094 | U1963 | U1827 | U1762 | U1701 | U1568 | U1498 | U1435 | U1435 |
| U     | U     | U2095 | U2095 | U1964 | U1828 | U1763 | U1702 | U1569 | U1499 | U1436 | U1436 |
| U     | U     | U2096 | U2096 | U1965 | U1829 | U1764 | U1703 | U1570 | U1500 | U1437 | U1437 |
| U     | U     | U2097 | U2097 | U1966 | U1830 | U1765 | U1704 | U1571 | U1501 | U1438 | U1438 |
| U     | U     | U2098 | U2098 | U1967 | U1831 | U1766 | U1705 | U1572 | U1502 | U1439 | U1439 |
| U     | U     | U2099 | U2099 | U1968 | U1832 | U1767 | U1706 | U1573 | U1503 | U1440 | U1440 |
| U     | U     | U2100 | U2100 | U1969 | U1833 | U1768 | U1707 | U1574 | U1504 | U1441 | U1441 |
| U     | U     | U2101 | U2101 | U1970 | U1834 | U1769 | U1708 | U1575 | U1505 | U1442 | U1442 |
| U     | U     | U2102 | U2102 | U1971 | U1835 | U1770 | U1709 | U1576 | U1506 | U1443 | U1443 |
| U     | U     | U2103 | U2103 | U1972 | U1836 | U1771 | U1710 | U1577 | U1507 | U1444 | U1444 |
| U     | U     | U2104 | U2104 | U1973 | U1837 | U1772 | U1711 | U1578 | U1508 | U1445 | U1445 |
| U     | U     | U2105 | U2105 | U1974 | U1838 | U1773 | U1712 | U1579 | U1509 | U1446 | U1446 |
| U     | U     | U2106 | U2106 | U1975 | U1839 | U1774 | U1713 | U1580 | U1510 | U1447 | U1447 |
| U     | U     | U2107 | U2107 | U1976 | U1840 | U1775 | U1714 | U1581 | U1511 | U1448 | U1448 |
| U     | U     | U2108 | U2108 | U1977 | U1841 | U1776 | U1715 | U1582 | U1512 | U1449 | U1449 |
| U     | U     | U2109 | U2109 | U1978 | U1842 | U1777 | U1716 | U1583 | U1513 | U1450 | U1450 |
| U     | U     | U2110 | U2110 | U1979 | U1843 | U1778 | U1717 | U1584 | U1514 | U1451 | U1451 |
| U     | U     | U2111 | U2111 | U1980 | U1844 | U1779 | U1718 | U1585 | U1515 | U1452 | U1452 |
| U     | U     | U2112 | U2112 | U1981 | U1845 | U1780 | U1719 | U1586 | U1516 | U1453 | U1453 |
| U     | U     | U2113 | U2113 | U1982 | U1846 | U1781 | U1720 | U1587 | U1517 | U1454 | U1454 |
| U     | U     | U2114 | U2114 | U1983 | U1847 | U1782 | U1721 | U1588 | U1518 | U1455 | U1455 |
| U     | U     | U2115 | U2115 | U1984 | U1848 | U1783 | U1722 | U1589 | U1519 | U1456 | U1456 |
| U     | U     | U2116 | U2116 | U1985 | U1849 | U1784 | U1723 | U1590 | U1520 | U1457 | U1457 |
| U     | U     | U2117 | U2117 | U1986 | U1850 | U1785 | U1724 | U1591 | U1521 | U1458 | U1458 |
| U     | U     | U2118 | U2118 | U1987 | U1851 | U1786 | U1725 | U1592 | U1522 | U1459 | U1459 |
| U     | U     | U2119 | U2119 | U1988 | U1852 | U1787 | U1726 | U1593 | U1523 | U1460 | U1460 |
| U     | U     | U2120 | U2120 | U1989 | U1853 | U1788 | U1727 | U1594 | U1524 | U1461 | U1461 |
| U     | U     | U2121 | U2121 | U1990 | U1854 | U1789 | U1728 | U1595 | U1525 | U1462 | U1462 |
| U     | U     | U2122 | U2122 | U1991 | U1855 | U1790 | U1729 | U1596 | U1526 | U1463 | U1463 |
| U     | U     | U2123 | U2123 | U1992 | U1856 | U1791 | U1730 | U1597 | U1527 | U1464 | U1464 |
| U     | U     | U2124 | U2124 | U1993 | U1857 | U1792 | U1731 | U1598 | U1528 | U1465 | U1465 |
| U     | U     | U2125 | U2125 | U1994 | U1858 | U1793 | U1732 | U1599 | U1529 | U1466 | U1466 |
| U     | U     | U2126 | U2126 | U1995 | U1859 | U1794 | U1733 | U1600 | U1530 | U1467 | U1467 |
| U     | U     | U2127 | U2127 | U1996 | U1860 | U1795 | U1734 | U1601 | U1531 | U1468 | U1468 |
| U     | U     | U2128 | U2128 | U1997 | U1861 | U1796 | U1735 | U1602 | U1532 | U1469 | U1469 |
| U     | U     | U2129 | U2129 | U1998 | U1862 | U1797 | U1736 | U1603 | U1533 | U1470 | U1470 |
| U     | U     | U2130 | U2130 | U1999 | U1863 | U1798 | U1737 | U1604 | U1534 | U1471 | U1471 |
| U     | U     | U2131 | U2131 | U2000 | U1864 | U1799 | U1738 | U1605 | U1535 | U1472 | U1472 |
| U     | U     | U2132 | U2132 | U2001 | U1865 | U1800 | U1739 | U1606 | U1536 | U1473 | U1473 |
| U     | U     | U2133 | U2133 | U2002 | U1866 | A1801 | U1740 | U1607 | U1537 | U1474 | U1474 |
| U     | U     | U2134 | U2134 | U2003 | U1867 | A1802 | U1741 | U1608 | U1538 | U1475 | U1475 |
| U     | U     | U2135 | U2135 | U2004 | U1868 | A1803 | U1742 | U1609 | U1539 | U1476 | U1476 |
| U     | U     | U2136 | U2136 | U2005 | U1869 | A1804 | U1743 | U1610 | U1540 | U1477 | U1477 |
| U     | U     | U2137 | U2137 | U2006 | U1870 | A1805 | U1744 | U1611 | U1541 | U1478 | U1478 |
| U     | U     | U2138 | U2138 | U2007 | U1871 | A1806 | U1745 | U1612 | U1542 | U1479 | U1479 |
| U     | U     | U2139 | U2139 | U2008 | U1872 | A1807 | U1746 | U1613 | U1543 | U1480 | U1480 |
| U     |       |       |       |       |       |       |       |       |       |       |       |

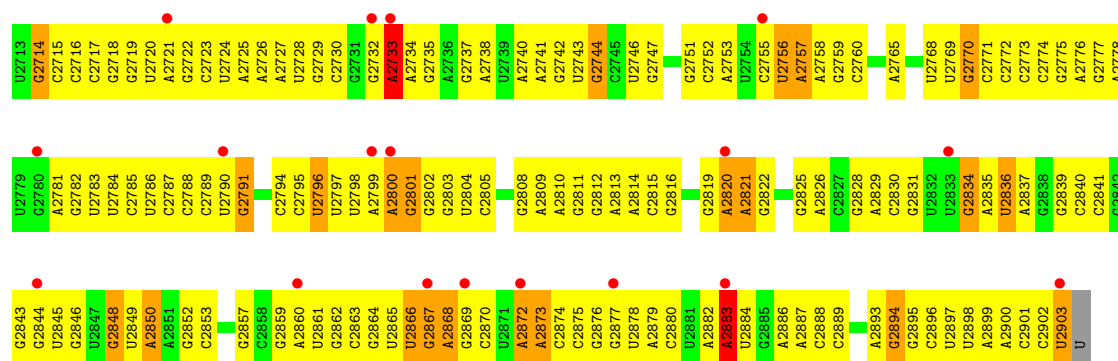




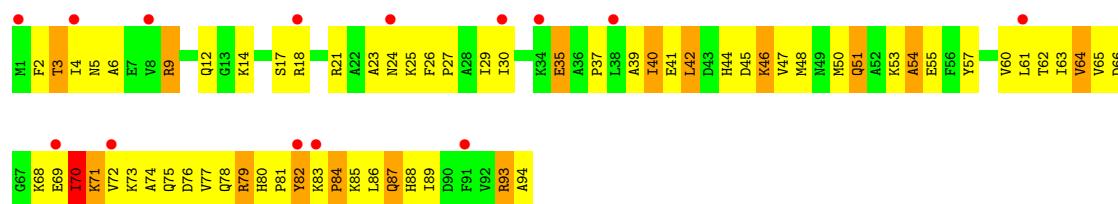
|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| A1794 | C1795 | U1796 | G1797 | U1798 | G1799 | C1800 | A1801 | A1802 | A1803 | A1808 | A1809 | A1810 | A1811 | A1812 | A1813 | A1814 | A1815 | C1816 | C1817 | A1818 | A1819 | A1820 | A1821 | C1822 | A1823 | A1824 | A1825 | A1826 | A1827 | A1828 | A1829 | C1830 | A1831 | A1832 | C1833 | C1838 | U1841 | G1842 | C1843 | C1844 | G1845 | A1846 | A1847 | A1848 | A1843 | A1853 | A1854 | U1855 | U1856 | A1857 | A1858 | G1862 | G1863 | U1864 | U1865 |       |       |       |
| G1731 | G1732 | G1733 | G1734 | G1735 | U1736 | G1737 | G1738 | G1739 | G1740 | G1741 | U1742 | G1743 | A1744 | A1745 | A1746 | U1747 | C1748 | A1749 | G1750 | U1751 | G1752 | G1753 | A1754 | A1757 | U1758 | A1759 | C1760 | C1761 | A1762 | G1763 | C1764 | C1765 | G1766 | U1769 | G1770 | C1771 | A1772 | A1773 | U1774 | U1775 | G1776 | U1777 | U1778 | U1779 | A1780 | U1781 | A1784 | A1785 | A1786 | A1787 | C1788 | A1789 | C1790 | A1791 | G1792 | C1793 |       |       |
| G1666 | G1667 | A1668 | A1669 | C1670 | U1671 | A1672 | G1673 | G1674 | A1675 | A1676 | A1677 | A1678 | A1679 | U1680 | G1681 | G1682 | U1683 | A1684 | C1685 | C1686 | G1687 | G1688 | A1689 | A1690 | C1691 | G1695 | G1699 | A1700 | A1701 | C1704 | A1705 | C1706 | G1707 | C1708 | U1709 | G1710 | A1711 | U1712 | U1713 | U1714 | G1715 | U1716 | U1717 | A1718 | G1719 | U1720 | G1721 | A1722 | G1723 | A1724 | U1725 | C1726 | C1727 | U1728 | U1729 | C1730 |       |       |
| A1593 | U1594 | C1595 | A1596 | A1597 | A1598 | U1599 | C1600 | G1601 | U1602 | A1603 | C1606 | C1607 | A1608 | A1609 | A1610 | C1611 | C1612 | G1613 | A1616 | C1617 | G1623 | U1624 | A1630 | G1633 | A1634 | A1635 | U1636 | C1637 | C1638 | C1639 | A1640 | A1641 | G1642 | G1643 | C1644 | G1645 | C1646 | U1647 | U1648 | C1649 | A1650 | G1651 | A1654 | A1655 | C1656 | C1657 | C1658 | C1659 | G1660 | G1661 | U1662 | A1665 |       |       |       |       |       |       |
| G1530 | C1531 | A1532 | C1533 | U1534 | A1535 | C1536 | G1537 | G1538 | U1539 | G1540 | C1541 | U1542 | G1543 | A1544 | A1545 | C1546 | C1547 | A1548 | A1549 | C1550 | A1551 | A1552 | A1553 | U1554 | G1555 | C1556 | C1557 | U1558 | U1559 | C1560 | C1561 | C1562 | U1563 | C1564 | C1565 | A1566 | G1567 | G1568 | A1569 | A1570 | A1571 | A1572 | U1576 | C1577 | U1578 | A1579 | A1580 | G1581 | C1582 | A1583 | C1584 | A1586 | U1589 | A1590 | A1591 | C1592 |       |       |
| C1463 | G1464 | U1465 | U1466 | U1467 | U1468 | A1469 | A1470 | G1471 | U1474 | U1475 | U1476 | A1477 | G1478 | G1479 | C1480 | U1481 | C1482 | G1483 | U1484 | U1485 | U1486 | U1487 | C1488 | C1489 | A1490 | C1493 | A1494 | U1495 | U1496 | U1497 | C1498 | C1499 | G1500 | G1501 | A1502 | A1503 | A1504 | A1505 | U1506 | C1507 | A1508 | A1509 | G1510 | G1511 | U1512 | U1513 | G1514 | A1515 | G1516 | G1517 | A1524 | A1525 | C1526 | U1527 | A1528 | G1529 |       |       |
| U1402 | A1403 | C1404 | U1405 | U1406 | G1407 | U1408 | U1409 | G1410 | U1411 | U1412 | A1413 | A1414 | U1415 | G1416 | C1417 | U1418 | A1419 | A1420 | G1421 | G1422 | G1423 | C1424 | G1425 | A1426 | A1427 | C1428 | G1429 | G1430 | A1431 | C1432 | C1433 | A1434 | C1437 | U1438 | A1439 | U1440 | G1441 | U1442 | U1443 | U1444 | G1445 | C1446 | C1447 | G1448 | A1449 | C1450 | C1451 | G1452 | A1453 | C1454 | G1455 | G1456 | U1457 | U1458 | G1459 | U1460 | C1461 | C1462 |
| C1330 | G1331 | G1332 | G1337 | U1340 | G1341 | C1345 | U1346 | A1347 | C1348 | C1351 | U1352 | A1353 | A1354 | C1355 | G1356 | C1357 | G1358 | A1359 | C1360 | G1361 | A1365 | A1366 | A1367 | C1368 | G1369 | C1370 | C1371 | U1372 | A1373 | C1374 | U1375 | U1379 | G1380 | G1381 | C1382 | U1383 | A1384 | A1385 | C1386 | A1387 | C1388 | G1389 | U1390 | U1391 | U1394 | A1395 | U1396 | U1397 | C1398 | C1399 | U1400 | G1401 |       |       |       |       |       |       |
| U1267 | A1268 | A1269 | C1270 | U1271 | U1272 | U1273 | A1274 | U1275 | A1276 | U1277 | C1278 | G1281 | U1282 | A1284 | A1285 | A1286 | A1287 | C1288 | C1289 | C1290 | C1291 | G1292 | C1293 | U1294 | C1295 | C1296 | C1297 | C1298 | C1299 | G1300 | A1301 | A1302 | C1306 | A1307 | A1308 | G1309 | G1310 | G1311 | U1312 | U1313 | C1314 | C1315 | U1316 | C1317 | U1318 | C1319 | C1320 | A1321 | C1322 | C1323 | U1324 | U1325 | U1326 | A1327 | U1329 |       |       |       |
| U1199 | C1200 | G1201 | G1202 | U1203 | A1204 | A1205 | G1206 | G1210 | C1211 | G1212 | A1213 | A1214 | G1215 | G1216 | U1217 | G1218 | U1219 | C1220 | C1221 | U1222 | G1223 | U1224 | G1225 | G1228 | A1230 | G1235 | U1236 | A1237 | U1240 | A1241 | U1242 | C1243 | A1244 | G1245 | A1246 | G1248 | U1249 | G1250 | C1251 | G1252 | A1253 | A1254 | U1255 | G1256 | G1259 | U1260 | C1261 | A1262 | U1263 | A1264 | A1265 | G1266 |       |       |       |       |       |       |
| G1137 | G1138 | G1139 | C1140 | U1141 | A1142 | A1143 | A1144 | C1145 | A1146 | A1147 | U1148 | C1149 | C1150 | A1151 | C1152 | C1153 | G1154 | A1155 | G1157 | C1161 | G1162 | G1163 | C1164 | A1165 | C1166 | C1167 | G1168 | A1169 | C1170 | G1171 | C1172 | U1173 | U1174 | C1175 | U1176 | G1177 | C1178 | C1179 | U1180 | U1181 | G1182 | U1183 | U1184 | G1185 | C1186 | G1187 | U1188 | A1189 | G1190 | U1191 | G1192 | G1193 | U1194 | C1195 | C1196 | G1197 | U1198 |       |
| A1069 | A1070 | G1071 | C1072 | A1073 | C1076 | A1077 | U1080 | U1081 | U1082 | U1083 | A1084 | A1085 | A1086 | A1087 | A1088 | A1089 | A1090 | G1091 | C1092 | G1093 | U1094 | U1097 | A1098 | C1099 | C1100 | U1101 | U1105 | G1106 | C1107 | U1108 | C1109 | G1110 | A1111 | G1112 | U1113 | C1114 | G1115 | C1116 | C1117 | C1118 | U1119 | G1120 | C1121 | G1125 | G1128 | U1129 | U1130 | G1131 | U1132 | A1133 | A1134 | C1135 | G1136 |       |       |       |       |       |
| G1002 | C1005 | U1006 | C1007 | A1008 | A1009 | A1010 | G1011 | U1012 | C1013 | A1014 | U1018 | U1019 | A1020 | A1021 | A1022 | U1023 | G1024 | G1025 | G1026 | A1027 | A1028 | C1029 | C1030 | A1031 | A1032 | U1033 | G1034 | U1035 | G1038 | A1039 | A1040 | G1041 | G1042 | C1043 | A1046 | A1047 | A1048 | C1049 | A1050 | G1051 | C1052 | G1055 | A1056 | A1057 | U1058 | G1059 | U1060 | U1061 | G1062 | G1063 | C1064 | U1065 | G1068 |       |       |       |       |       |



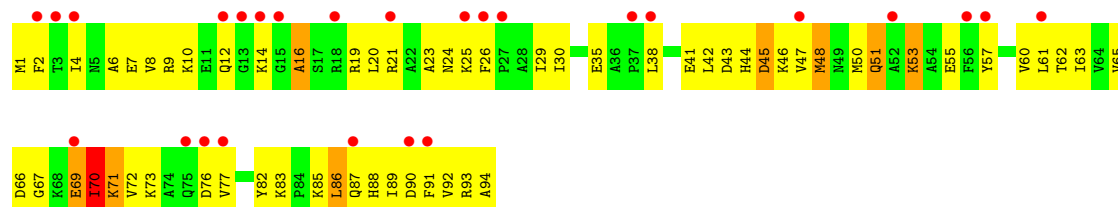
|       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| U2650 | C2581 | C2515 | G2444 | G2379 | A2314 | G2250 | U2187 | G2067 | A1998 | U1931 | A1866 |
| C2651 | U2585 | A2516 | A2448 | C2380 | G2315 | G2251 | U2188 | U2068 | C1999 | A1932 | G1867 |
| C2652 | U2586 | A2518 | U2449 | A2381 | G2316 | G2252 | U2189 | A2069 | C2000 | G1933 | C1868 |
| A2654 | U2587 | A2519 | A2450 | G2382 | A2317 | G2253 | G2190 | G2070 | C2001 | C1934 | C1869 |
| A2657 | G2588 | C2520 | A2451 | U2383 | G2318 | G2256 | A2191 | C2072 | G2002 | G1935 | C1870 |
| C2658 | A2589 | C2521 | G2455 | C2385 | U2320 | U2257 | U2192 | C2073 | C2008 | A1936 | A1871 |
| G2659 | C2591 | U2552 | G2456 | A2386 | U2321 | C2258 |       | C2074 | A2009 | A1937 | A1872 |
| A2665 | C2592 | G2526 | U2457 | U2387 | A2322 | U2259 | U2196 | U2075 | A2010 | A1938 | G1873 |
| C2666 | G2593 | C2527 | G2458 | A2388 | G2323 | C2260 | C2197 | U2076 | G2010 | U1939 | G1874 |
| G2667 | C2594 | U2528 | A2459 | U2390 | U2324 | C2261 | A2198 | A2077 | U2011 | U1940 | G1875 |
| A2662 | G2595 | G2529 | U2460 | U2391 | G2325 | U2262 | A2199 | C2078 | G2012 | C1941 | A1876 |
| G2663 | A2596 | A2530 | A2461 | A2392 | C2326 | G2266 | C2200 | C2079 | U2016 | G1942 | A1877 |
| G2664 | C2597 | A2531 | A2462 | U2393 | A2327 | A2266 | G2201 | A2080 | U2017 | U1943 | G1878 |
| A2665 | A2598 | G2532 | C2463 | U2394 | U2328 | A2267 | U2202 | U2081 | U2018 | U1944 | C1879 |
| C2666 | G2599 | U2533 | G2464 | C2395 | A2329 | A2268 | U2203 | A2082 | G2019 | G1945 | U1880 |
| G2667 | A2600 | U2534 | C2465 | G2396 | G2330 | G2269 | U2197 | U2083 | A2020 | U1946 | C1881 |
| A2668 | C2601 | A2534 | C2466 | U2397 | C2331 | A2270 | A2198 | C2084 | G2021 | G1947 | U1882 |
| G2669 | A2602 | G2535 | C2467 | G2397 | C2332 | G2271 | G2143 | U2085 | U2022 | G1948 | U1883 |
| A2670 | G2603 | U2537 | A2468 | U2398 | A2333 | U2272 | C2145 | U2086 | C2023 | G1949 | G1884 |
| G2671 | U2604 | C2538 | G2471 | G2400 | A2334 | A2273 | G2146 | G2087 | C2024 | G1950 | A1885 |
| G2672 | C2605 | C2539 | U2472 | U2401 | A2335 | A2274 | A2142 | A2088 | A2019 | U1951 | U1886 |
| A2673 | G2606 | C2540 | U2473 | U2402 | A2336 | G2275 | U2149 | C2089 | G2025 | A1952 | C1887 |
| G2674 | U2609 | A2541 | U2474 | C2403 | G2337 | G2276 | A2150 | A2090 | U2026 | G1953 | A1888 |
| C2675 | C2610 | U2542 | U2475 | U2404 | C2338 | G2277 | U2151 | C2091 | G2027 | G1954 | A1889 |
| G2676 | U2611 | A2543 | C2476 | G2405 | C2339 | A2278 | G2152 | U2092 | G2029 | U1955 | A1890 |
| G2677 | U2612 | G2544 | A2477 | A2406 | A2340 | G2279 | C2153 | A2093 | A2030 | U1956 | G1891 |
| A2678 | U2613 | U2545 | U2478 | A2407 | G2341 | G2280 | A2154 | G2094 | A2031 | C1957 | C1892 |
| G2679 | U2614 | U2546 | U2479 | U2408 | C2342 | A2281 | U2155 | C2095 | G2032 | G1958 | C1893 |
| C2680 | U2615 | U2547 | G2480 | G2410 | U2343 | G2282 | G2156 | A2096 | A2033 | G1959 | C1894 |
| G2681 | U2616 | U2548 | G2481 | G2411 | G2344 | A2283 | G2157 | U2097 | U2034 | G1964 | G1897 |
| A2682 | G2617 | C2551 | G2482 | A2412 | G2345 | A2284 | A     | U2098 | G2035 | C1965 | U1898 |
| C2683 | G2618 | U2552 | G2483 | G2413 | A2346 | A2285 | G     | U2099 | C2036 | A1966 | G1903 |
| G2684 | G2621 | U2553 | G2484 | U2414 | G2347 | G2286 | C     | G2100 | G2037 | C1967 | G1904 |
| C2685 | C2626 | U2554 | G2488 | G2415 | U2348 | A2287 | C     | A2101 | A2038 | G1970 | C1905 |
| G2686 | G2627 | U2555 | U2489 | G2416 | G2349 | A2288 | G     | G2102 | U2039 | U1971 | G1906 |
| U2689 | C2628 | C2556 | G2490 | G2417 | C2350 | G2289 | A     | C2103 | G2040 | G1972 | C1909 |
| C2691 | G2630 | G2557 | U2491 | C2420 | G2351 | G2290 | C     | G2104 | A2042 | A1977 | A1912 |
| G2692 | G2631 | C2558 | U2492 | G2421 | G2352 | U2291 | C     | U2105 | C2043 | U1978 | A1913 |
| C2693 | A2632 | U2560 | C2496 | U2423 | G2353 | U2292 | U     | A2108 | G2045 | U1979 | C1914 |
| G2694 | G2633 | A2561 | A2497 | C2424 | G2354 | G2293 | A     | U2109 | C2046 | G1980 | U1915 |
| U2695 | A2634 | U2562 | C2498 | A2425 | G2355 | A2297 | A     | U     | G2048 | A1981 | A1916 |
| C2696 | G2635 | U2563 | C2499 | A2426 | G2356 | U2298 | U     | G     | A2051 | G1985 | U1917 |
| U2698 | C2636 | A2564 | U2500 | G2427 | G2357 | U2299 | A     | A     | A2052 | C1986 | A1918 |
| C2699 | U2637 | A2565 | C2501 | G2428 | G2358 | C2300 | C     | G     | G2053 | A1987 | A1919 |
| G2699 | G2638 | U2566 | G2502 | G2429 | G2359 | G2301 | A     | A     | A2054 | G1988 | C1920 |
| A2700 | A2639 | G2567 | A2503 | A2430 | G2360 | G2304 | C     | U     | C2055 | G1921 | G1922 |
| U2701 | G2640 | U2568 | U2504 | G2431 | G2361 | U2305 | U     | U     | G2056 | U1916 | G1923 |
| C2704 | G2641 | G2569 | G2505 | A2434 | G2362 | A2306 | A     | A     | A2060 | G1989 | C1924 |
| A2705 | U2642 | U2570 | U2506 | A2435 | G2363 | G2307 | G     | G     | G2061 | U1991 | U1925 |
| U2706 | G2643 | U2571 | C2507 | U2438 | G2364 | U2245 | U     | U     | A2062 | G1992 | C1926 |
| G2707 | A2644 | C2572 | G2508 | A2439 | G2365 | U2246 | G     | G     | G2063 | G1993 | U1926 |
| C2708 | G2645 | A2573 | G2509 | C2440 | G2366 | G2247 | A     | A     | C2064 | C1994 | A1927 |
| G2709 | G2646 | G2574 | U2511 | C2441 | A2376 | G2248 | G     | G     | C2065 | U1995 | A1928 |
| U2710 | U2647 | C2575 | C2512 | U2442 | A2377 | U2249 | G     | G     | C2066 | C1996 | C1929 |
| A2711 | G2648 | U2578 | U2514 | C2443 | A2378 |       | A     | A     |       | C1997 | G1930 |



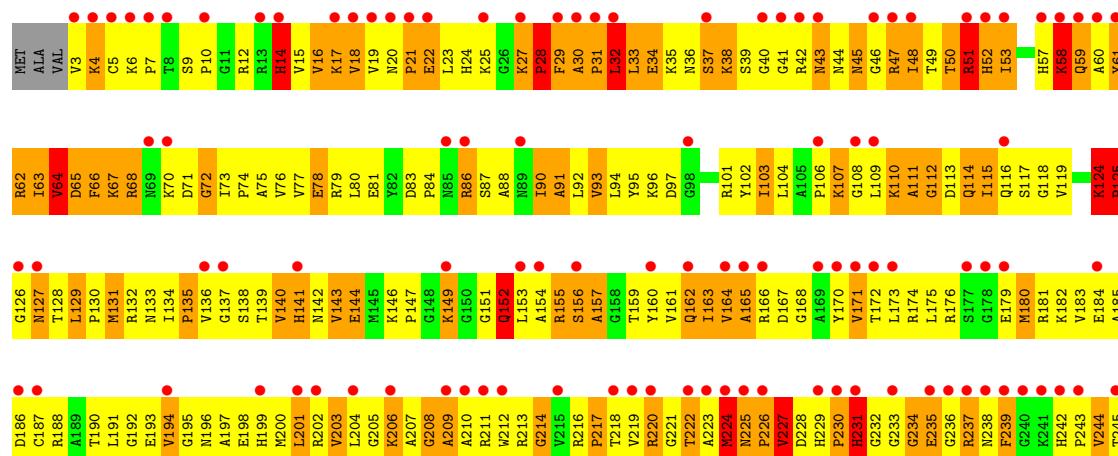
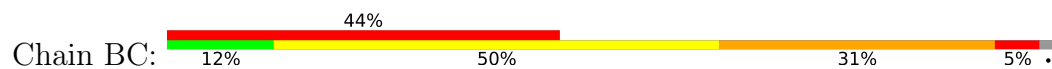
• Molecule 24: 50S RIBOSOMAL PROTEIN L25

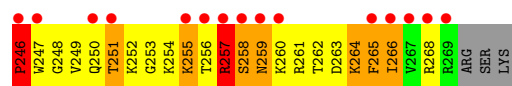


• Molecule 24: 50S RIBOSOMAL PROTEIN L25

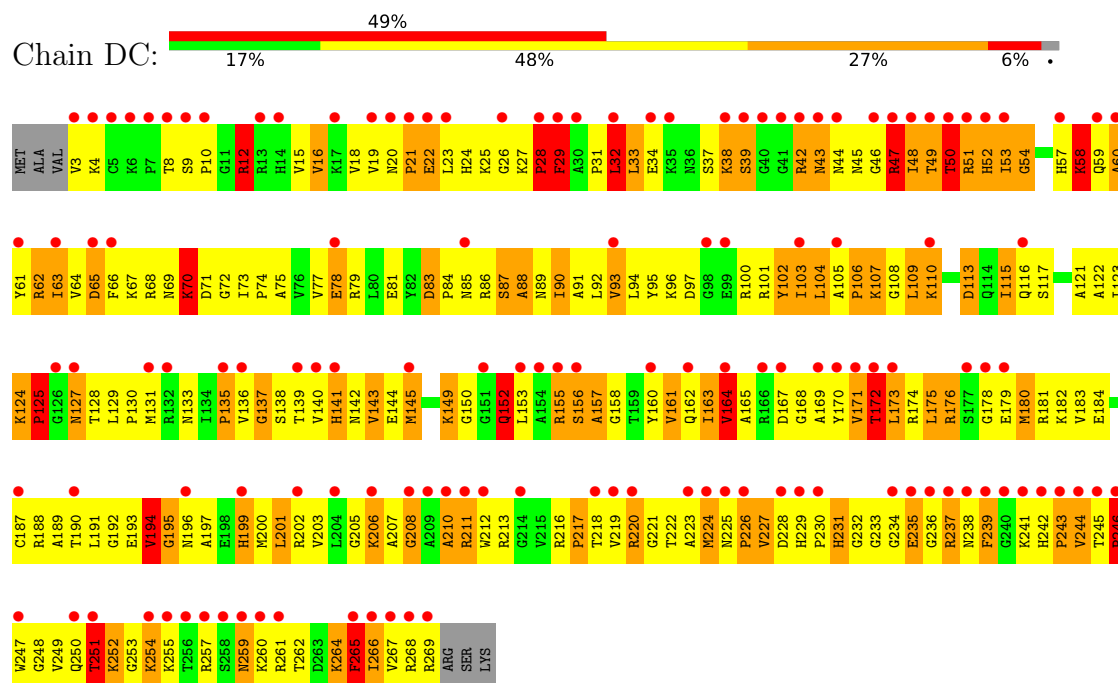


• Molecule 25: 50S RIBOSOMAL PROTEIN L2

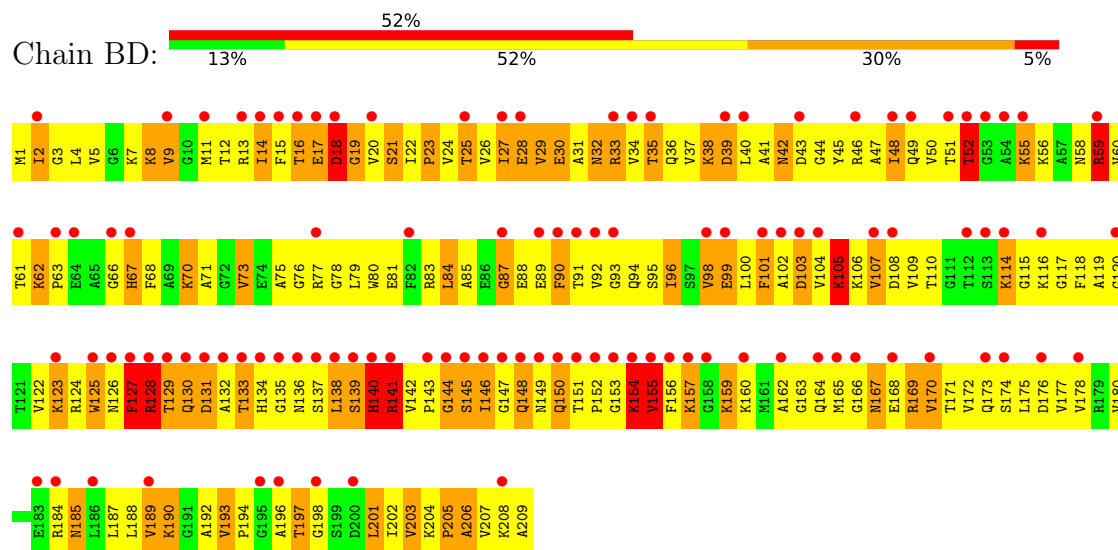




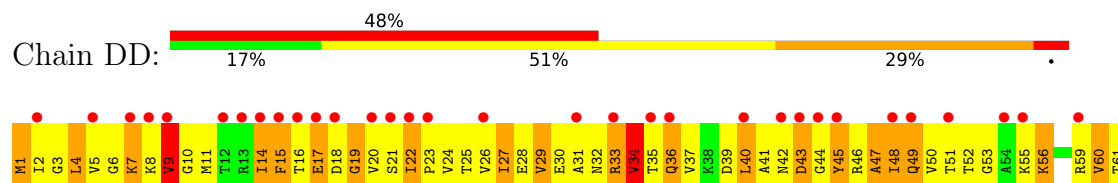
• Molecule 25: 50S RIBOSOMAL PROTEIN L2

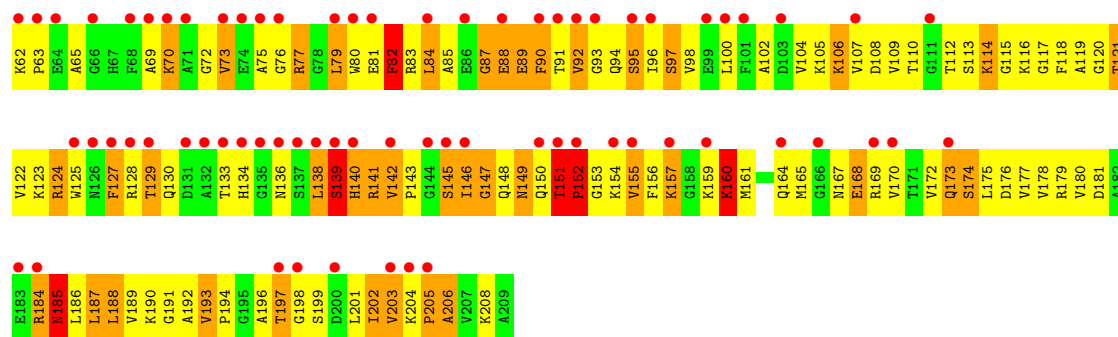


• Molecule 26: 50S RIBOSOMAL PROTEIN L3

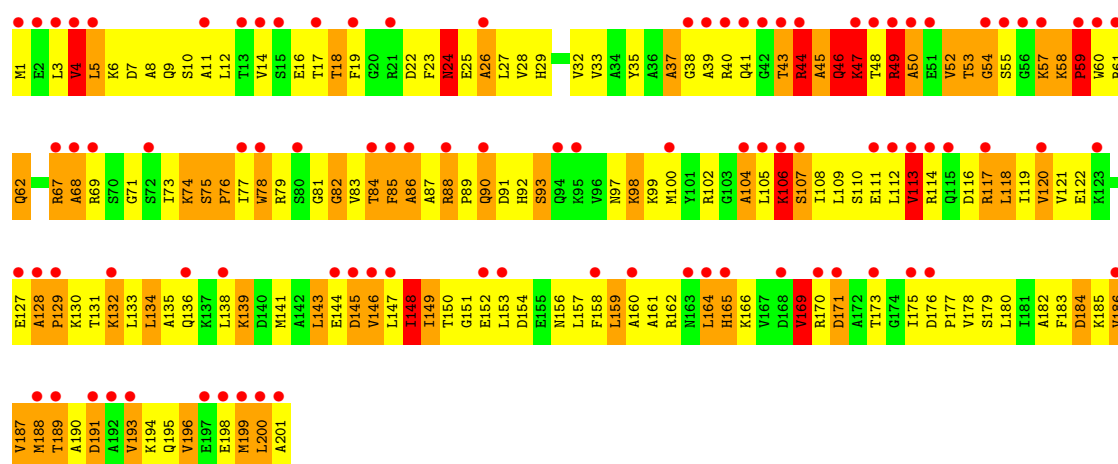
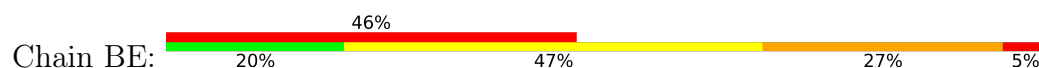


• Molecule 26: 50S RIBOSOMAL PROTEIN L3

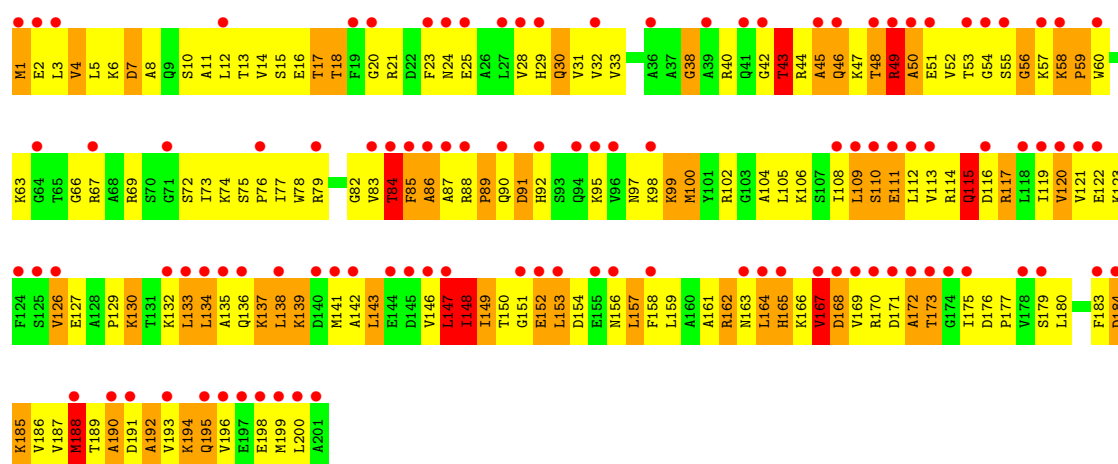




• Molecule 27: 50S RIBOSOMAL PROTEIN L4

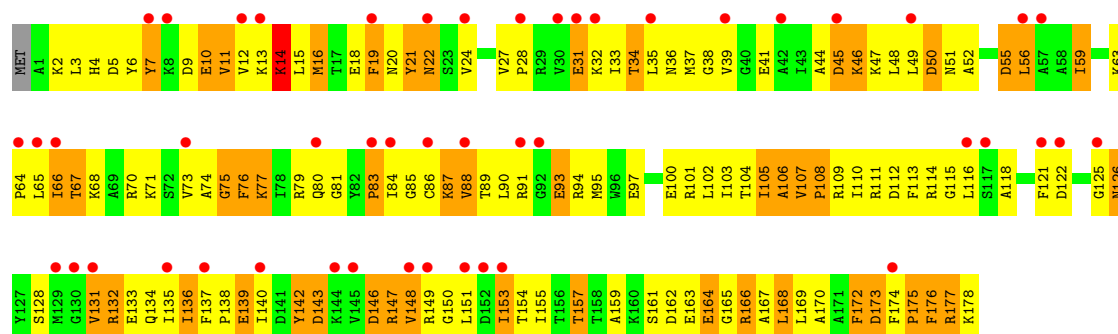


• Molecule 27: 50S RIBOSOMAL PROTEIN L4

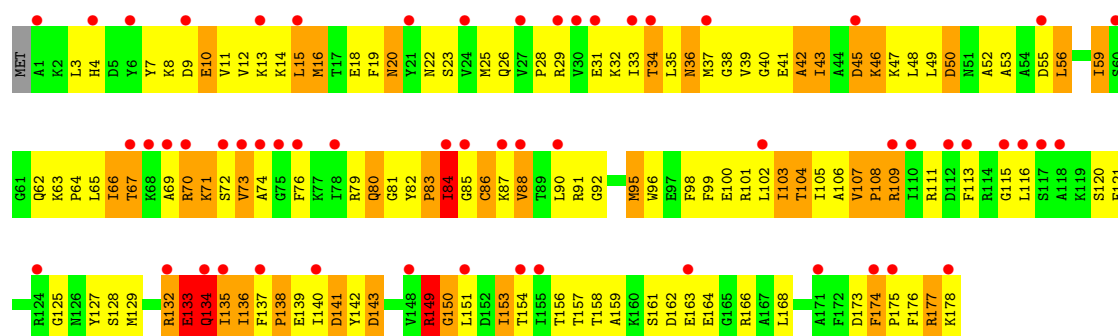


• Molecule 28: 50S RIBOSOMAL PROTEIN L5

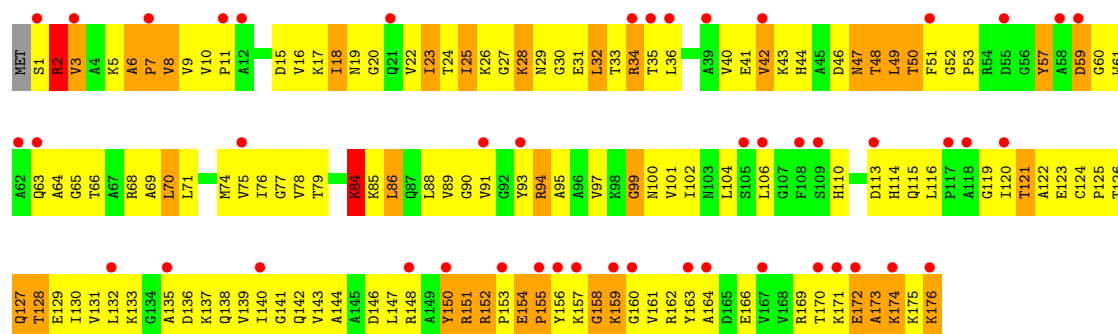




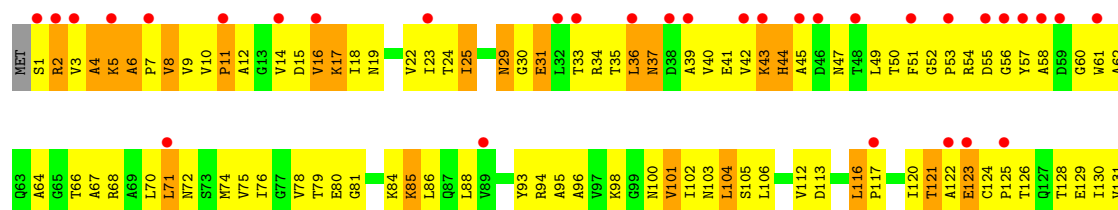
• Molecule 28: 50S RIBOSOMAL PROTEIN L5

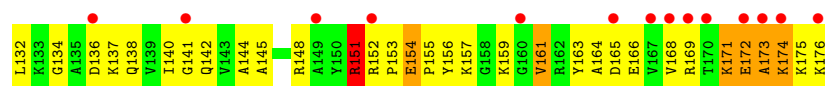


• Molecule 29: 50S RIBOSOMAL PROTEIN L6

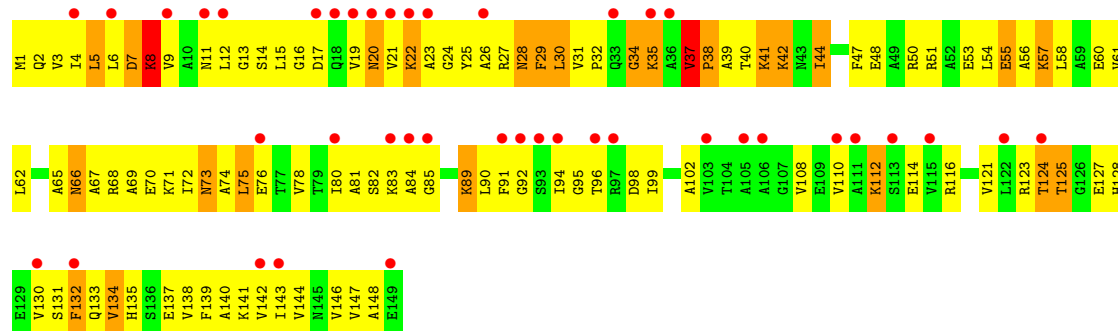


• Molecule 29: 50S RIBOSOMAL PROTEIN L6

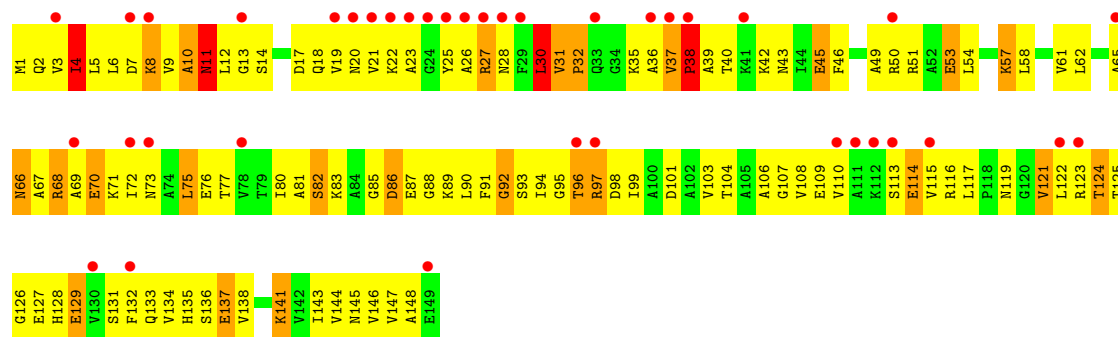




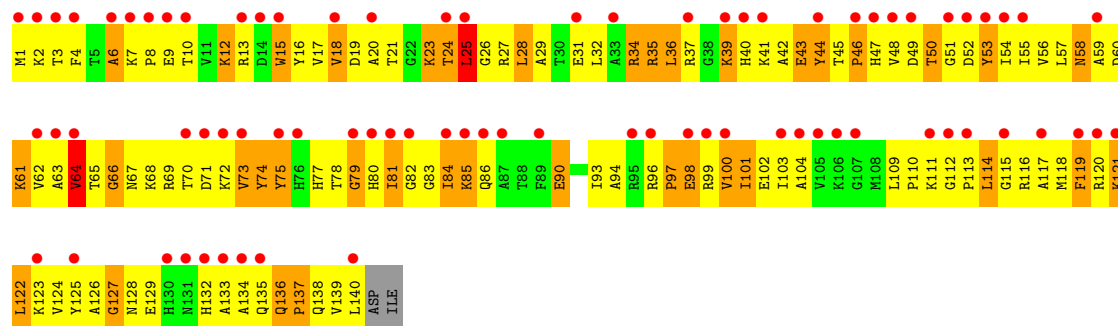
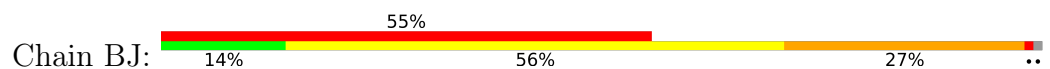
• Molecule 30: 50S RIBOSOMAL PROTEIN L9



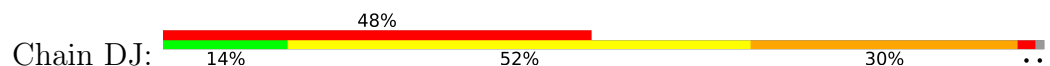
• Molecule 30: 50S RIBOSOMAL PROTEIN L9

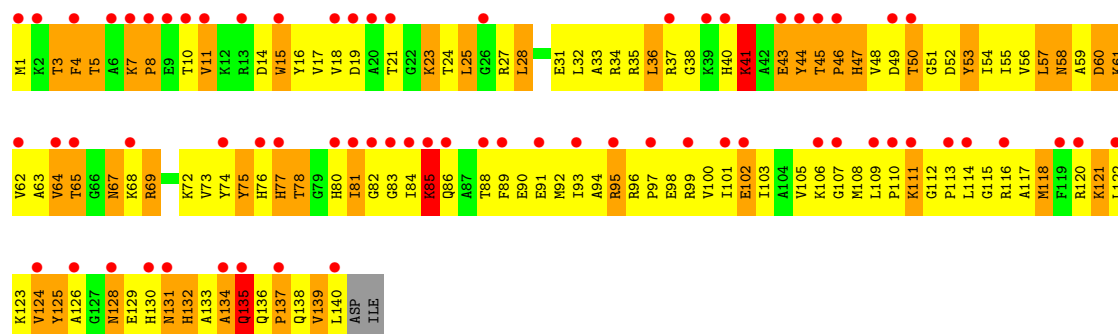


• Molecule 31: 50S RIBOSOMAL PROTEIN L13

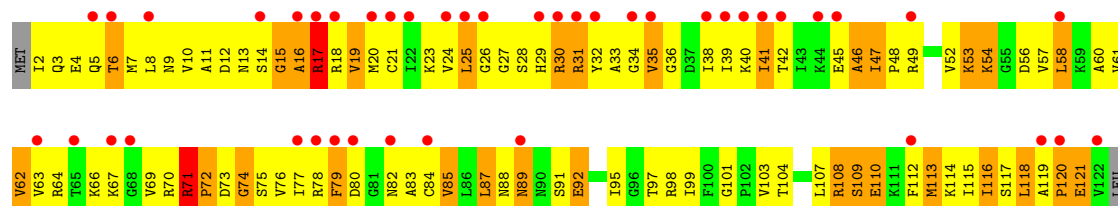
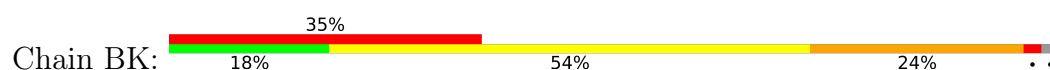


• Molecule 31: 50S RIBOSOMAL PROTEIN L13

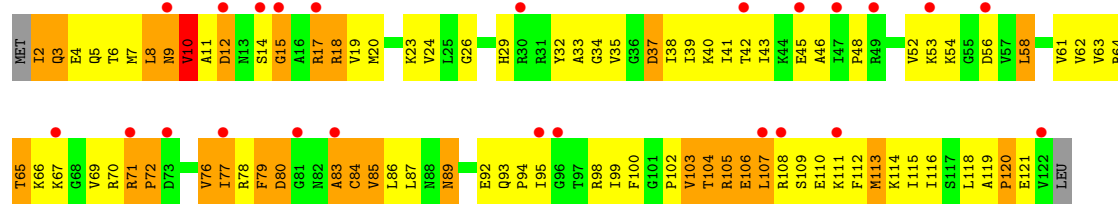




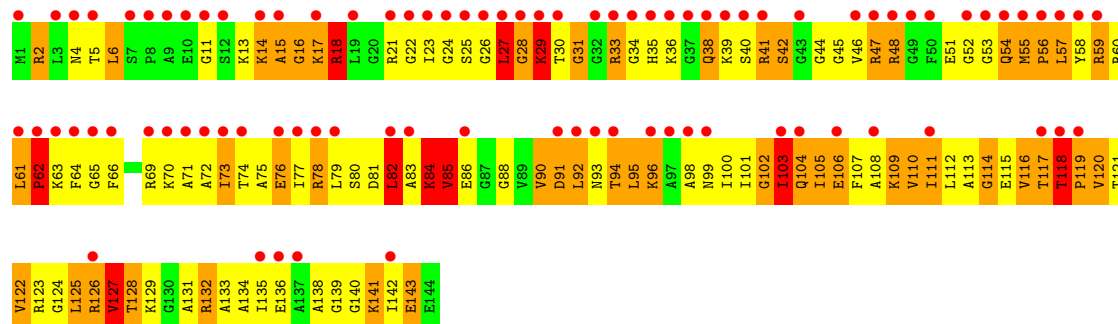
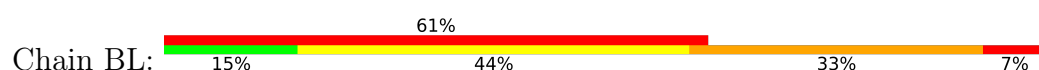
• Molecule 32: 50S RIBOSOMAL PROTEIN L14



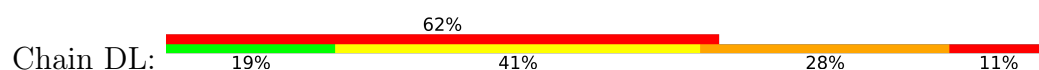
• Molecule 32: 50S RIBOSOMAL PROTEIN L14

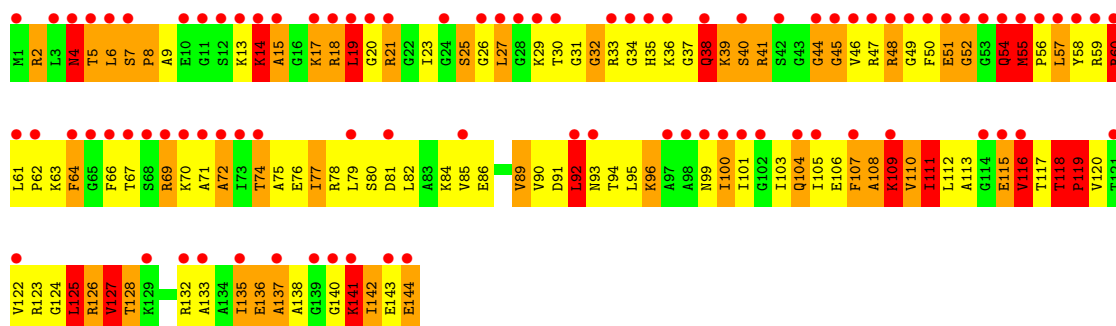


• Molecule 33: 50S RIBOSOMAL PROTEIN L15

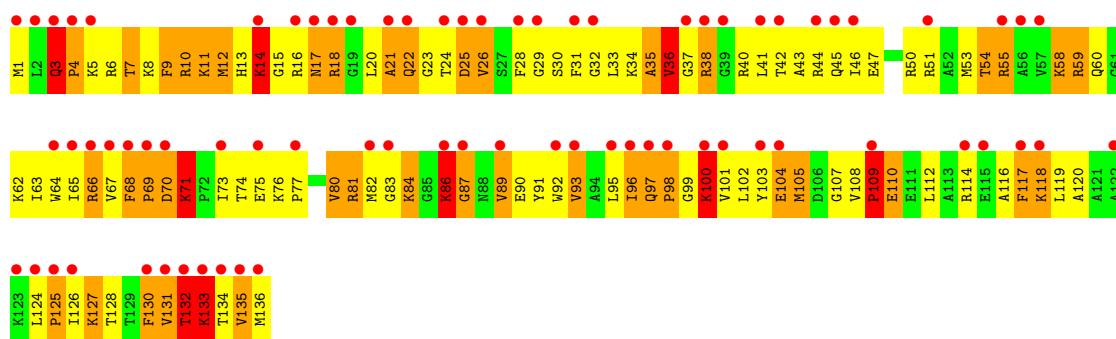
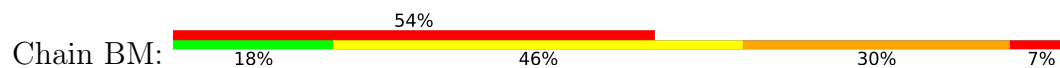


• Molecule 33: 50S RIBOSOMAL PROTEIN L15

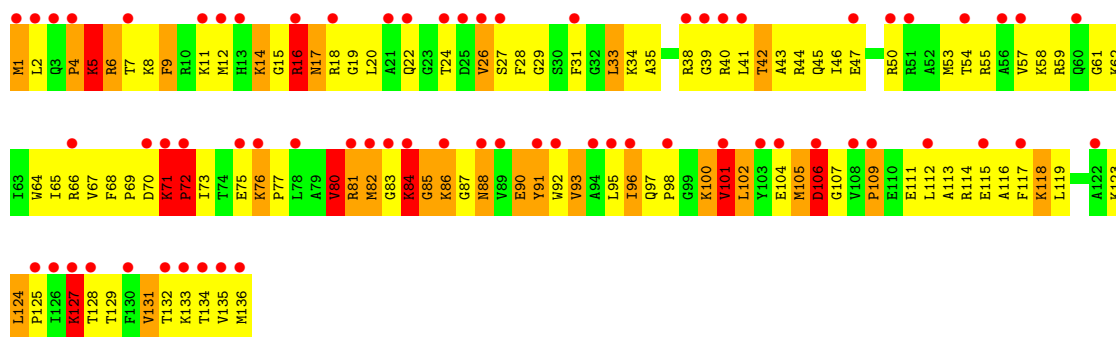




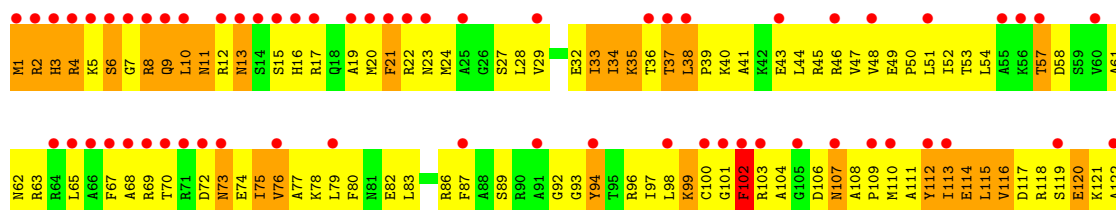
• Molecule 34: 50S RIBOSOMAL PROTEIN L16



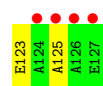
• Molecule 34: 50S RIBOSOMAL PROTEIN L16



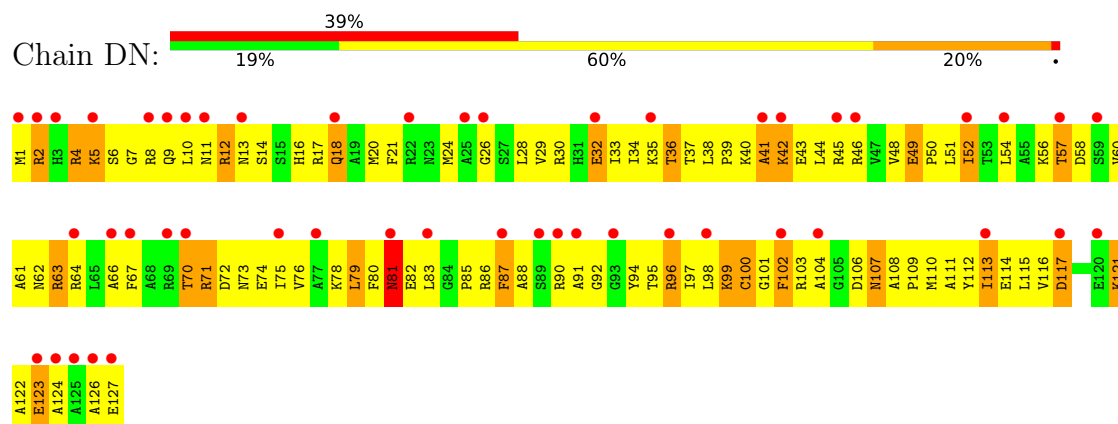
• Molecule 35: 50S RIBOSOMAL PROTEIN L17



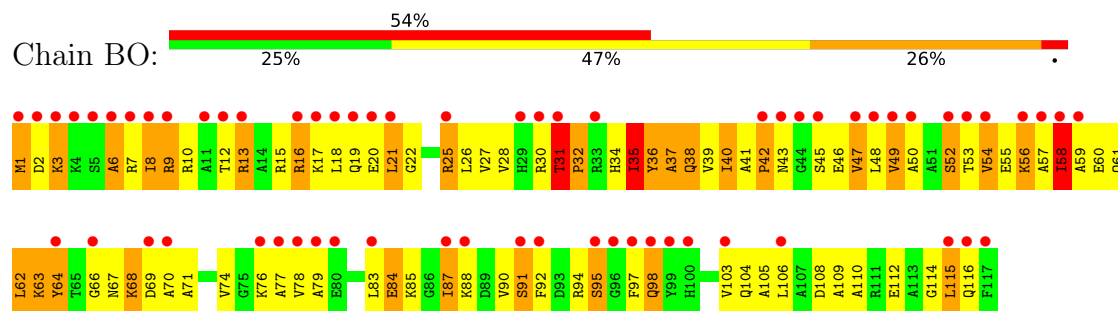




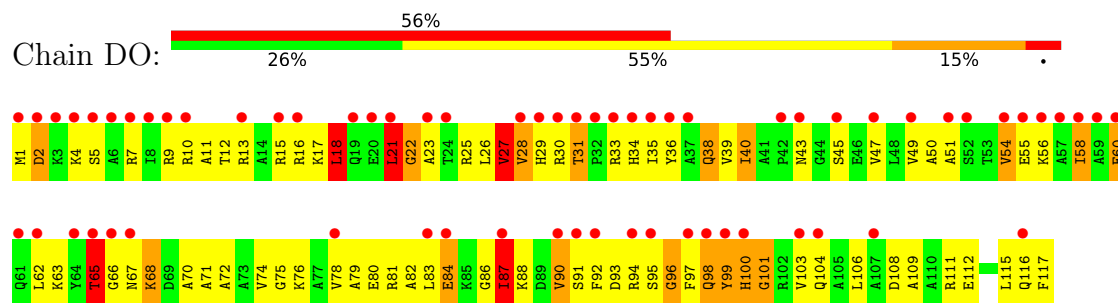
• Molecule 35: 50S RIBOSOMAL PROTEIN L17



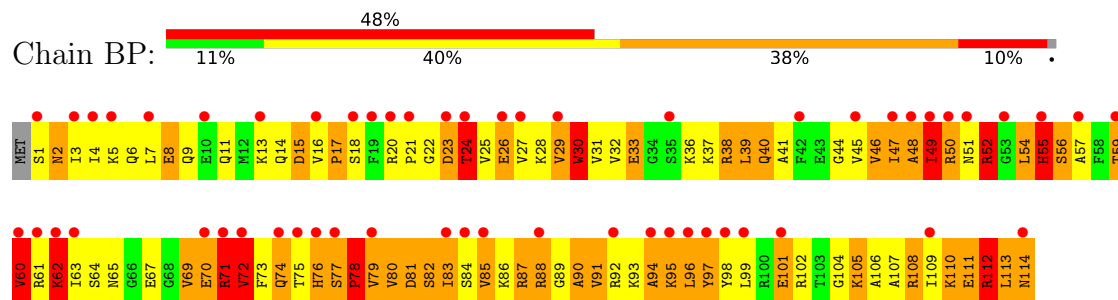
• Molecule 36: 50S RIBOSOMAL PROTEIN L18



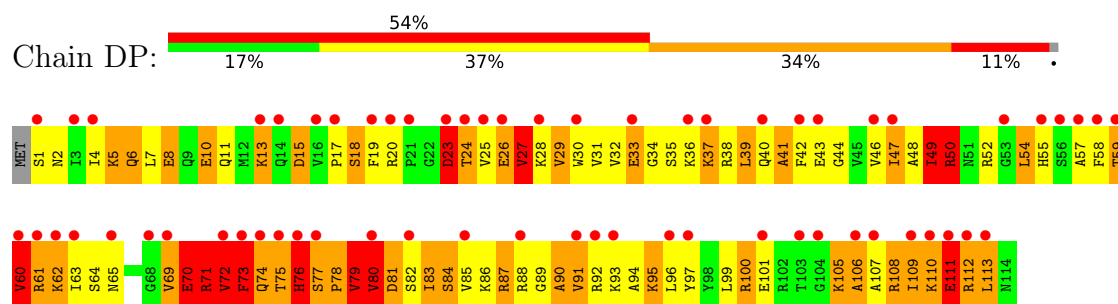
• Molecule 36: 50S RIBOSOMAL PROTEIN L18



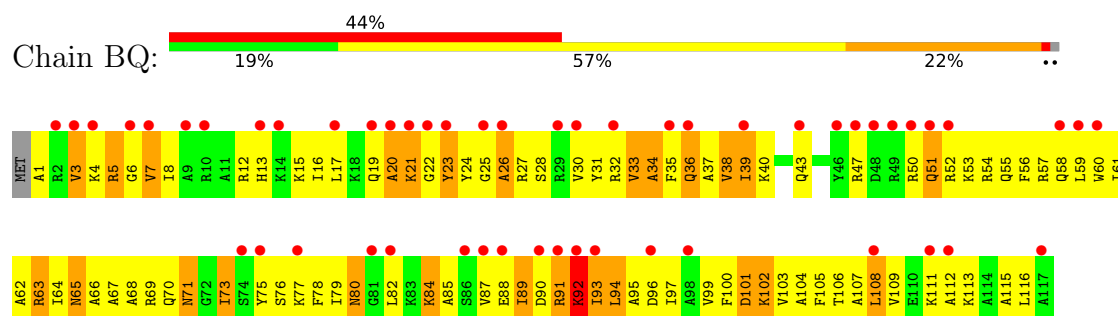
• Molecule 37: 50S RIBOSOMAL PROTEIN L19



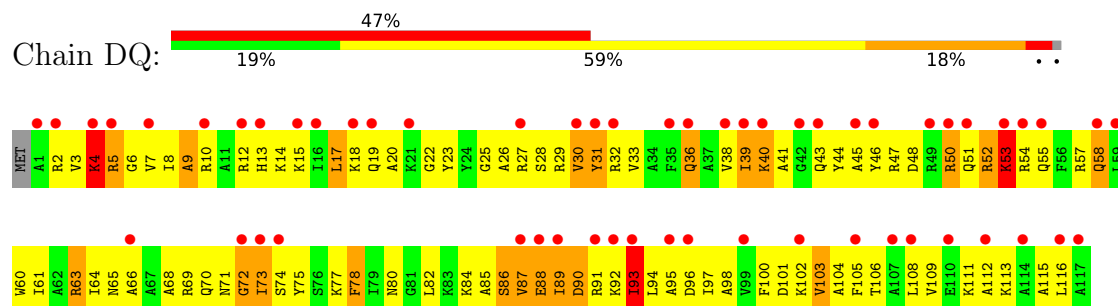
• Molecule 37: 50S RIBOSOMAL PROTEIN L19



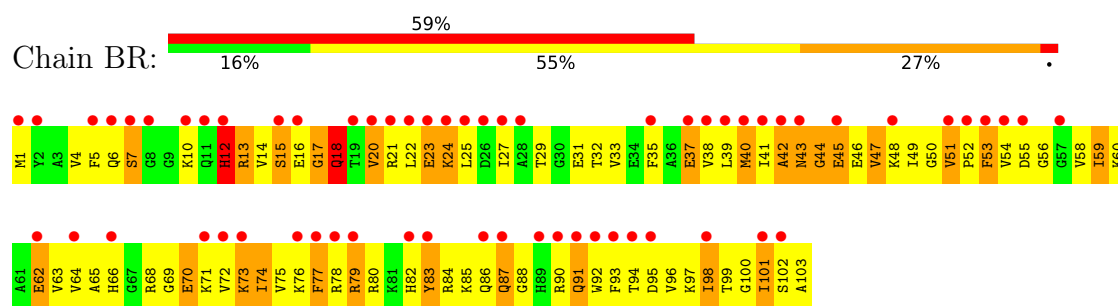
• Molecule 38: 50S RIBOSOMAL PROTEIN L20



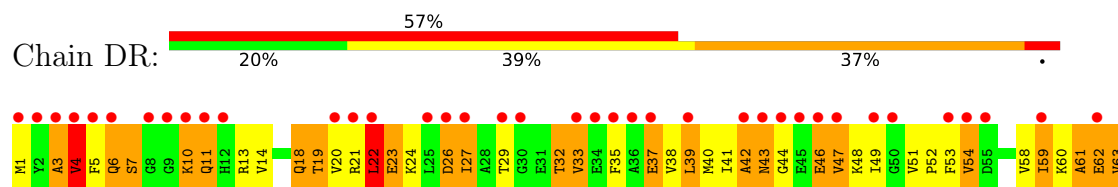
• Molecule 38: 50S RIBOSOMAL PROTEIN L20

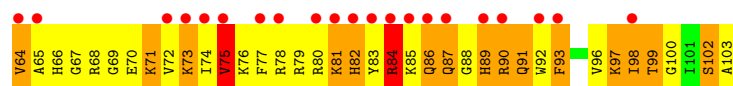


• Molecule 39: 50S RIBOSOMAL PROTEIN L21

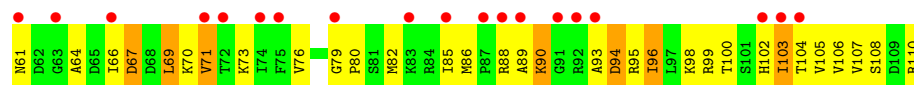
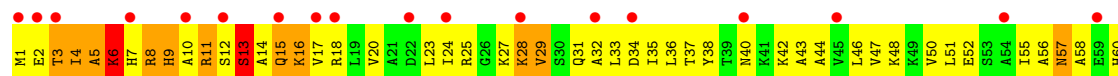


• Molecule 39: 50S RIBOSOMAL PROTEIN L21

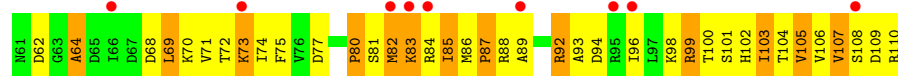
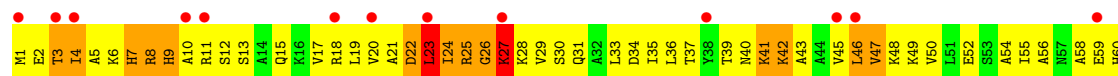




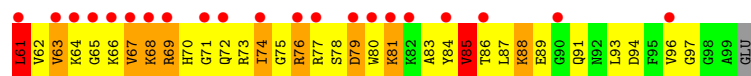
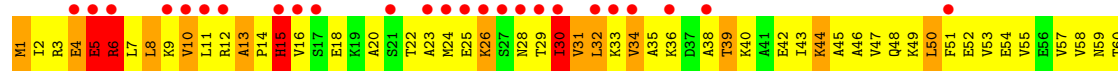
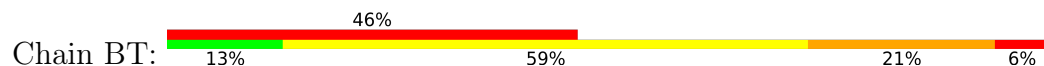
• Molecule 40: 50S RIBOSOMAL PROTEIN L22



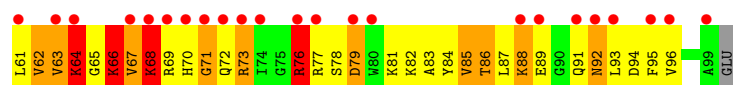
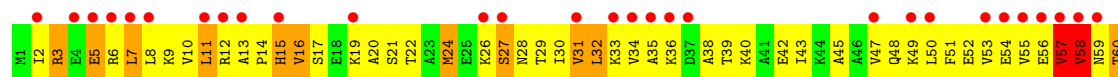
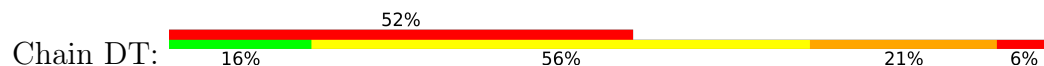
• Molecule 40: 50S RIBOSOMAL PROTEIN L22



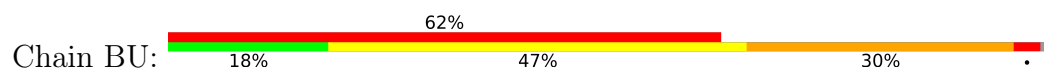
• Molecule 41: 50S RIBOSOMAL PROTEIN L23

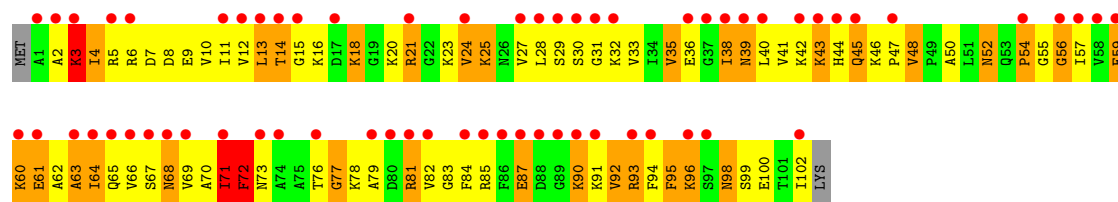


• Molecule 41: 50S RIBOSOMAL PROTEIN L23

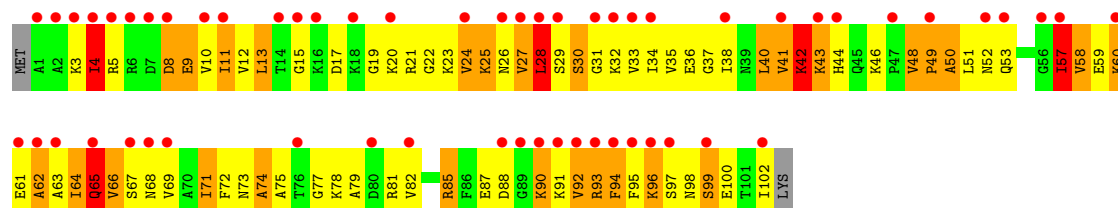
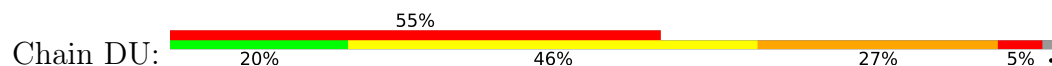


• Molecule 42: 50S RIBOSOMAL PROTEIN L24

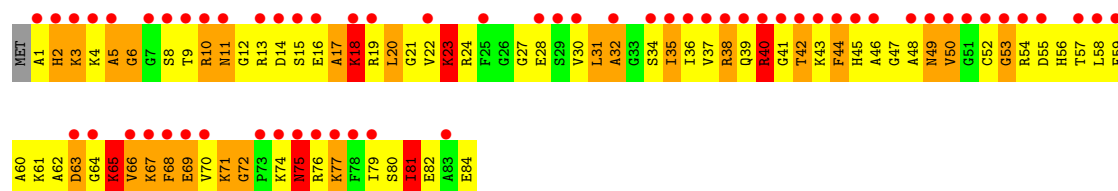
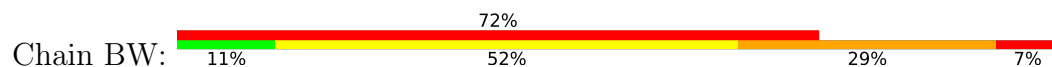




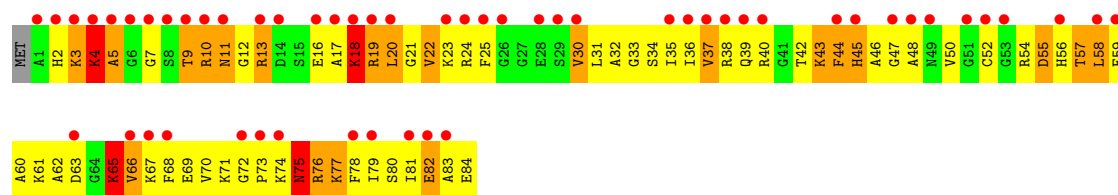
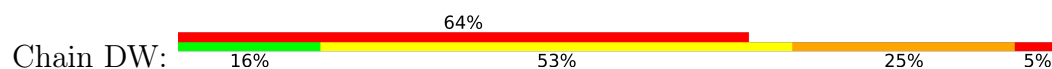
• Molecule 42: 50S RIBOSOMAL PROTEIN L24



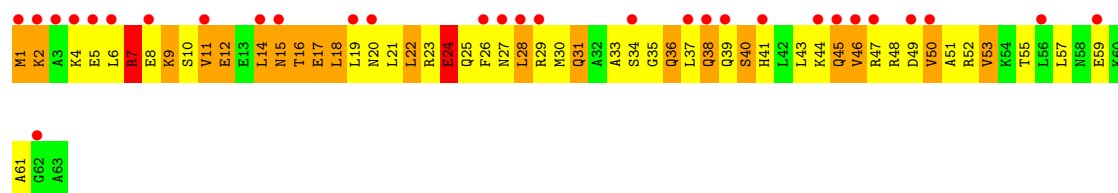
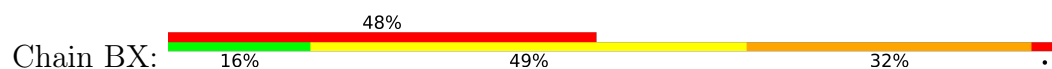
• Molecule 43: 50S RIBOSOMAL PROTEIN L27



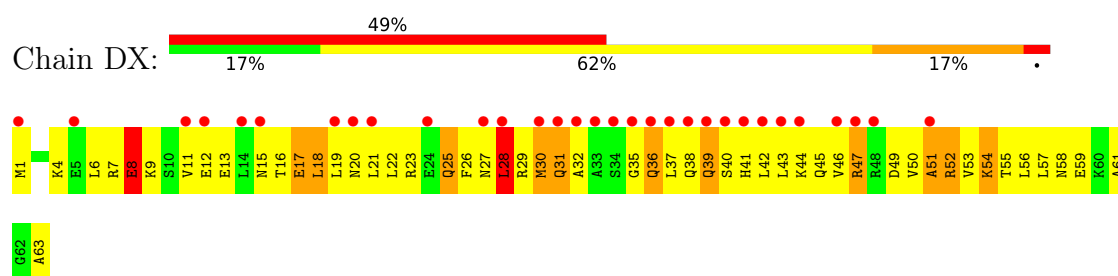
• Molecule 43: 50S RIBOSOMAL PROTEIN L27



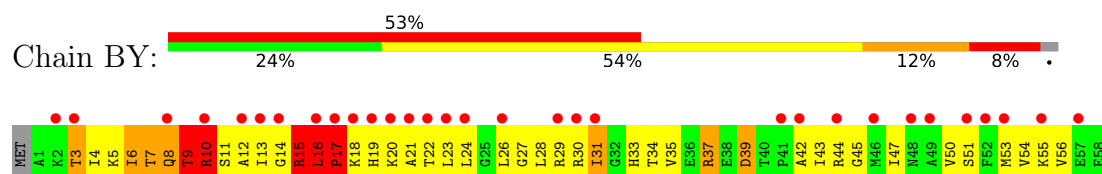
• Molecule 44: 50S RIBOSOMAL PROTEIN L29



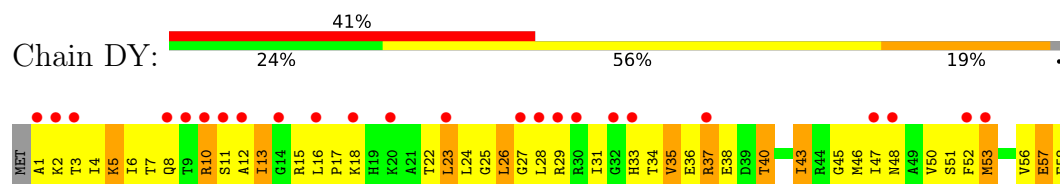
• Molecule 44: 50S RIBOSOMAL PROTEIN L29



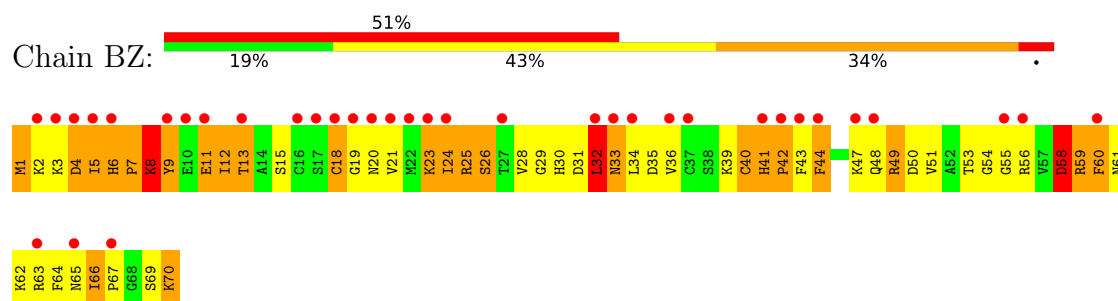
- Molecule 45: 50S RIBOSOMAL PROTEIN L30



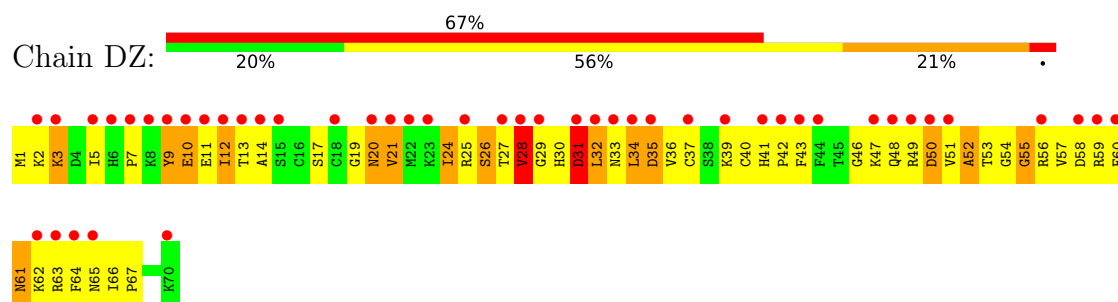
- Molecule 45: 50S RIBOSOMAL PROTEIN L30



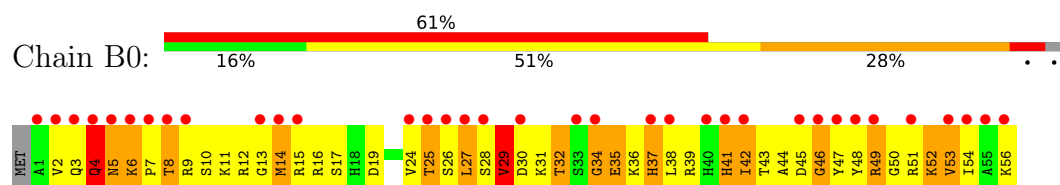
- Molecule 46: 50S RIBOSOMAL PROTEIN L31



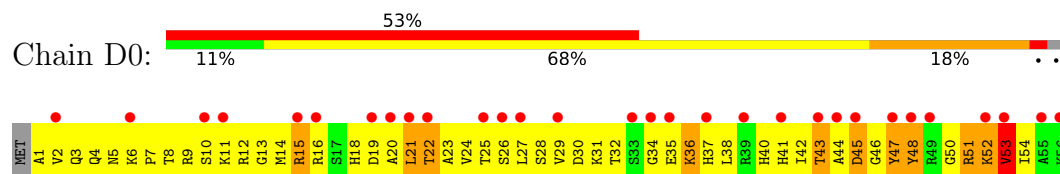
- Molecule 46: 50S RIBOSOMAL PROTEIN L31



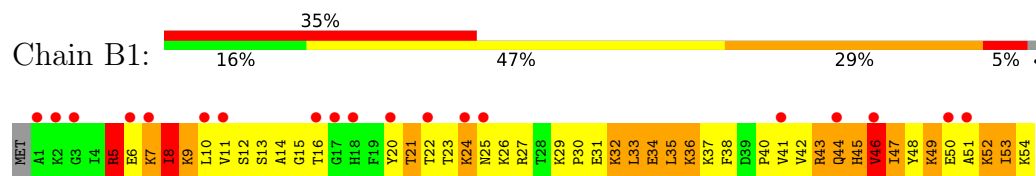
- Molecule 47: 50S RIBOSOMAL PROTEIN L32



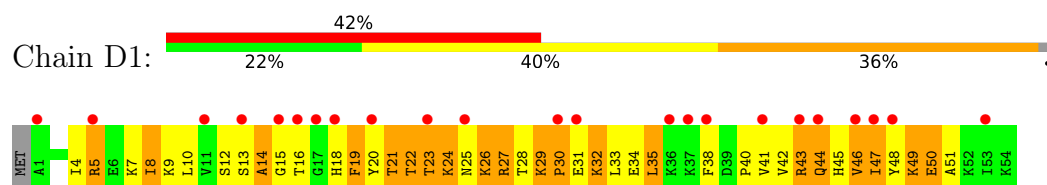
## ● Molecule 47: 50S RIBOSOMAL PROTEIN L32



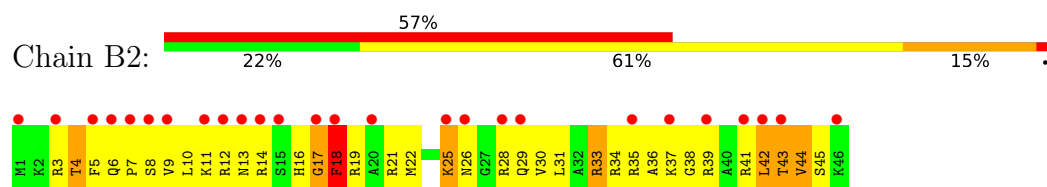
## ● Molecule 48: 50S RIBOSOMAL PROTEIN L33



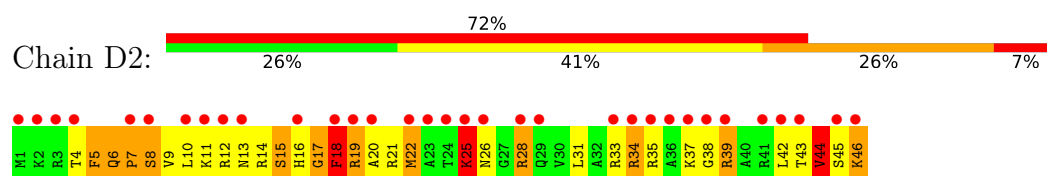
## ● Molecule 48: 50S RIBOSOMAL PROTEIN L33



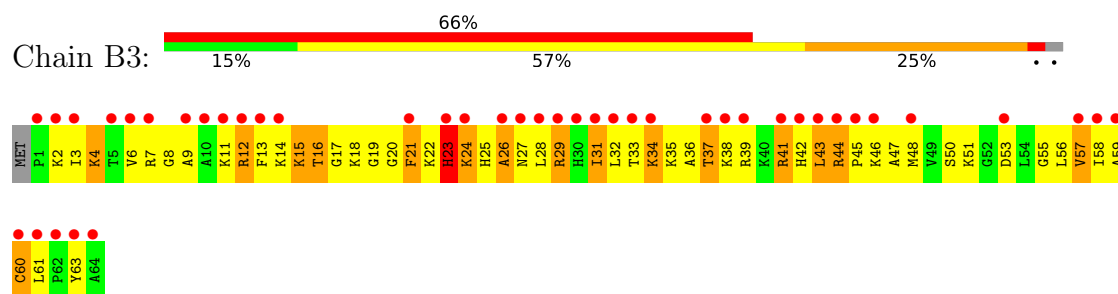
## ● Molecule 49: 50S RIBOSOMAL PROTEIN L34



## ● Molecule 49: 50S RIBOSOMAL PROTEIN L34

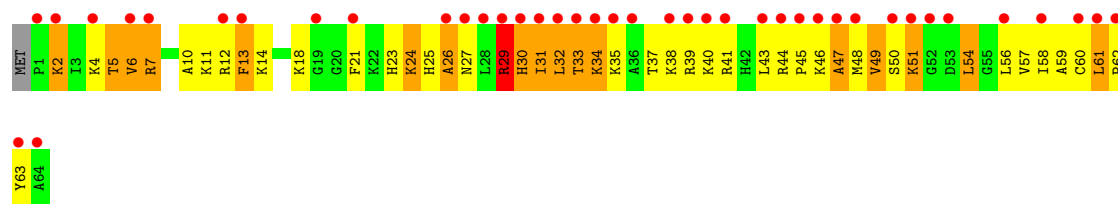


## ● Molecule 50: 50S RIBOSOMAL PROTEIN L35

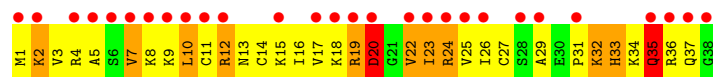
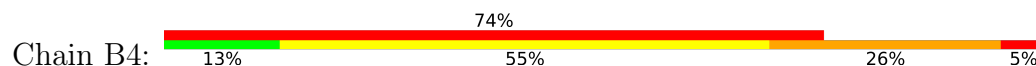


## ● Molecule 50: 50S RIBOSOMAL PROTEIN L35

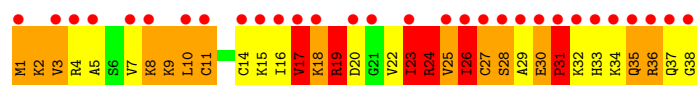
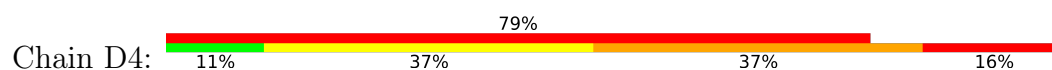




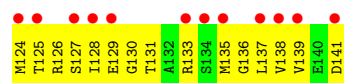
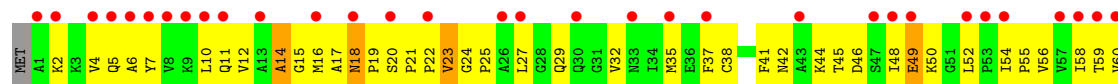
• Molecule 51: 50S RIBOSOMAL PROTEIN L36



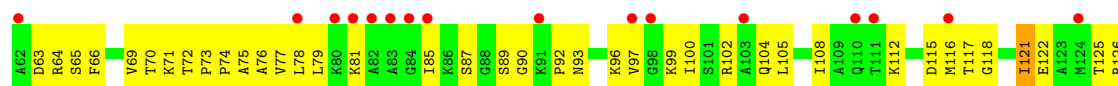
• Molecule 51: 50S RIBOSOMAL PROTEIN L36



• Molecule 52: 50S RIBOSOMAL PROTEIN L11



• Molecule 52: 50S RIBOSOMAL PROTEIN L11



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 208.85Å 379.20Å 739.28Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 70.00 – 3.46<br>70.00 – 3.54                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 91.6 (70.00-3.46)<br>93.1 (70.00-3.54)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.14                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.56 (at 3.58Å)                                             | Xtriage          |
| Refinement program                                                      | CNS                                                         | Depositor        |
| R, $R_{free}$                                                           | 0.279 , 0.331<br>0.286 , (Not available)                    | Depositor<br>DCC |
| $R_{free}$ test set                                                     | No test flags present.                                      | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 83.5                                                        | Xtriage          |
| Anisotropy                                                              | 0.179                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.26 , 62.9                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.86                                                        | EDS              |
| Total number of atoms                                                   | 284160                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 69.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.37% 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: KSG, 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   | AA    | 0.25         | 0/36762     | 0.55        | 14/57350 (0.0%) |
| 1   | CA    | 0.25         | 0/36762     | 0.56        | 18/57350 (0.0%) |
| 2   | AC    | 0.28         | 0/1651      | 0.72        | 1/2225 (0.0%)   |
| 2   | CC    | 0.28         | 0/1651      | 0.75        | 0/2225          |
| 3   | AD    | 0.26         | 0/1665      | 0.73        | 1/2227 (0.0%)   |
| 3   | CD    | 0.27         | 0/1665      | 0.74        | 0/2227          |
| 4   | AE    | 0.28         | 0/1118      | 0.75        | 0/1504          |
| 4   | CE    | 0.30         | 0/1118      | 0.75        | 0/1504          |
| 5   | AF    | 0.29         | 0/835       | 0.78        | 1/1128 (0.1%)   |
| 5   | CF    | 0.28         | 0/835       | 0.71        | 0/1128          |
| 6   | AG    | 0.27         | 0/1187      | 0.75        | 0/1591          |
| 6   | CG    | 0.27         | 0/1211      | 0.78        | 1/1624 (0.1%)   |
| 7   | AH    | 0.27         | 0/989       | 0.76        | 1/1326 (0.1%)   |
| 7   | CH    | 0.30         | 0/989       | 0.76        | 0/1326          |
| 8   | AI    | 0.27         | 0/1034      | 0.73        | 0/1375          |
| 8   | CI    | 0.28         | 0/1034      | 0.71        | 0/1375          |
| 9   | AJ    | 0.30         | 0/796       | 0.71        | 0/1077          |
| 9   | CJ    | 0.28         | 0/796       | 0.73        | 0/1077          |
| 10  | AK    | 0.28         | 0/893       | 0.75        | 0/1205          |
| 10  | CK    | 0.31         | 0/893       | 0.80        | 2/1205 (0.2%)   |
| 11  | AL    | 0.27         | 0/969       | 0.72        | 1/1300 (0.1%)   |
| 11  | CL    | 0.28         | 0/969       | 0.73        | 2/1300 (0.2%)   |
| 12  | AM    | 0.27         | 0/892       | 0.78        | 0/1193          |
| 12  | CM    | 0.27         | 0/884       | 0.76        | 0/1181          |
| 13  | AN    | 0.28         | 0/785       | 0.76        | 0/1043          |
| 13  | CN    | 0.26         | 0/785       | 0.66        | 0/1043          |
| 14  | AO    | 0.26         | 0/724       | 0.72        | 1/966 (0.1%)    |
| 14  | CO    | 0.26         | 0/724       | 0.78        | 1/966 (0.1%)    |
| 15  | AP    | 0.30         | 0/659       | 0.74        | 0/884           |
| 15  | CP    | 0.29         | 0/648       | 0.70        | 0/870           |
| 16  | AQ    | 0.26         | 0/657       | 0.67        | 0/881           |
| 16  | CQ    | 0.28         | 0/666       | 0.72        | 0/892           |

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5          |
| 17  | AR    | 0.30         | 0/462          | 0.75        | 0/621            |
| 17  | CR    | 0.30         | 0/462          | 0.73        | 0/621            |
| 18  | AS    | 0.26         | 0/652          | 0.71        | 0/877            |
| 18  | CS    | 0.26         | 0/660          | 0.72        | 0/888            |
| 19  | AT    | 0.29         | 0/671          | 0.79        | 0/888            |
| 19  | CT    | 0.29         | 0/671          | 0.71        | 0/888            |
| 20  | AB    | 0.31         | 1/1735 (0.1%)  | 0.77        | 1/2338 (0.0%)    |
| 20  | CB    | 0.29         | 0/1735         | 0.76        | 1/2338 (0.0%)    |
| 21  | AU    | 0.28         | 0/430          | 0.82        | 1/570 (0.2%)     |
| 21  | CU    | 0.28         | 0/430          | 0.95        | 2/570 (0.4%)     |
| 22  | BA    | 0.25         | 0/2803         | 0.53        | 0/4371           |
| 22  | DA    | 0.26         | 0/2803         | 0.56        | 0/4371           |
| 23  | BB    | 0.25         | 1/68314 (0.0%) | 0.56        | 13/106569 (0.0%) |
| 23  | DB    | 0.25         | 1/68314 (0.0%) | 0.56        | 19/106569 (0.0%) |
| 24  | BV    | 0.27         | 0/766          | 0.75        | 0/1025           |
| 24  | DV    | 0.28         | 0/766          | 0.74        | 0/1025           |
| 25  | BC    | 0.32         | 0/2092         | 0.90        | 7/2813 (0.2%)    |
| 25  | DC    | 0.30         | 0/2092         | 0.89        | 4/2813 (0.1%)    |
| 26  | BD    | 0.30         | 0/1586         | 0.79        | 3/2134 (0.1%)    |
| 26  | DD    | 0.30         | 0/1586         | 0.83        | 6/2134 (0.3%)    |
| 27  | BE    | 0.29         | 0/1571         | 0.86        | 6/2113 (0.3%)    |
| 27  | DE    | 0.29         | 0/1571         | 0.81        | 3/2113 (0.1%)    |
| 28  | BF    | 0.30         | 0/1444         | 0.99        | 8/1937 (0.4%)    |
| 28  | DF    | 0.28         | 0/1444         | 0.94        | 8/1937 (0.4%)    |
| 29  | BG    | 0.29         | 0/1343         | 0.80        | 1/1816 (0.1%)    |
| 29  | DG    | 0.27         | 0/1343         | 0.78        | 1/1816 (0.1%)    |
| 30  | BH    | 0.28         | 0/1122         | 0.77        | 2/1515 (0.1%)    |
| 30  | DH    | 0.28         | 0/1122         | 0.76        | 1/1515 (0.1%)    |
| 31  | BJ    | 0.29         | 0/1135         | 0.72        | 0/1529           |
| 31  | DJ    | 0.29         | 0/1135         | 0.88        | 3/1529 (0.2%)    |
| 32  | BK    | 0.29         | 0/939          | 0.95        | 3/1258 (0.2%)    |
| 32  | DK    | 0.28         | 0/939          | 1.00        | 9/1258 (0.7%)    |
| 33  | BL    | 0.33         | 0/1062         | 1.09        | 12/1413 (0.8%)   |
| 33  | DL    | 0.34         | 0/1062         | 1.11        | 11/1413 (0.8%)   |
| 34  | BM    | 0.33         | 0/1093         | 0.93        | 7/1460 (0.5%)    |
| 34  | DM    | 0.29         | 0/1093         | 0.88        | 4/1460 (0.3%)    |
| 35  | BN    | 0.30         | 0/1021         | 0.84        | 1/1364 (0.1%)    |
| 35  | DN    | 0.28         | 0/1021         | 0.79        | 2/1364 (0.1%)    |
| 36  | BO    | 0.28         | 0/910          | 0.83        | 5/1219 (0.4%)    |
| 36  | DO    | 0.28         | 0/910          | 0.76        | 2/1219 (0.2%)    |
| 37  | BP    | 0.31         | 0/929          | 1.21        | 11/1242 (0.9%)   |
| 37  | DP    | 0.31         | 0/929          | 1.23        | 11/1242 (0.9%)   |
| 38  | BQ    | 0.29         | 0/960          | 0.80        | 1/1278 (0.1%)    |

| Mol | Chain | Bond lengths |                 | Bond angles |                   |
|-----|-------|--------------|-----------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5           |
| 38  | DQ    | 0.30         | 0/960           | 0.83        | 0/1278            |
| 39  | BR    | 0.31         | 0/829           | 0.90        | 5/1107 (0.5%)     |
| 39  | DR    | 0.29         | 0/829           | 0.82        | 4/1107 (0.4%)     |
| 40  | BS    | 0.28         | 0/864           | 0.75        | 0/1156            |
| 40  | DS    | 0.28         | 0/864           | 0.79        | 2/1156 (0.2%)     |
| 41  | BT    | 0.29         | 0/784           | 0.74        | 2/1048 (0.2%)     |
| 41  | DT    | 0.30         | 0/784           | 0.85        | 4/1048 (0.4%)     |
| 42  | BU    | 0.27         | 0/787           | 0.77        | 0/1051            |
| 42  | DU    | 0.28         | 0/787           | 0.98        | 5/1051 (0.5%)     |
| 43  | BW    | 0.30         | 0/642           | 0.86        | 2/848 (0.2%)      |
| 43  | DW    | 0.28         | 0/642           | 0.78        | 2/848 (0.2%)      |
| 44  | BX    | 0.29         | 0/510           | 0.82        | 0/677             |
| 44  | DX    | 0.27         | 0/510           | 0.88        | 1/677 (0.1%)      |
| 45  | BY    | 0.30         | 0/453           | 0.68        | 0/605             |
| 45  | DY    | 0.30         | 0/453           | 0.78        | 0/605             |
| 46  | BZ    | 0.29         | 0/559           | 1.07        | 6/745 (0.8%)      |
| 46  | DZ    | 0.30         | 0/559           | 0.99        | 4/745 (0.5%)      |
| 47  | B0    | 0.34         | 0/450           | 0.85        | 2/599 (0.3%)      |
| 47  | D0    | 0.31         | 0/450           | 0.92        | 1/599 (0.2%)      |
| 48  | B1    | 0.30         | 0/448           | 0.74        | 0/594             |
| 48  | D1    | 0.30         | 0/448           | 0.67        | 0/594             |
| 49  | B2    | 0.30         | 0/380           | 0.78        | 1/498 (0.2%)      |
| 49  | D2    | 0.30         | 0/380           | 0.74        | 0/498             |
| 50  | B3    | 0.27         | 0/513           | 0.71        | 1/676 (0.1%)      |
| 50  | D3    | 0.28         | 0/513           | 0.74        | 0/676             |
| 51  | B4    | 0.29         | 0/303           | 0.86        | 0/397             |
| 51  | D4    | 0.30         | 0/303           | 0.78        | 0/397             |
| 52  | BI    | 0.32         | 0/1046          | 0.87        | 3/1410 (0.2%)     |
| 52  | DI    | 0.38         | 1/1046 (0.1%)   | 0.91        | 2/1410 (0.1%)     |
| All | All   | 0.26         | 4/306470 (0.0%) | 0.64        | 260/458101 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | AA    | 0                   | 14                  |
| 1   | CA    | 0                   | 16                  |
| 23  | BB    | 0                   | 41                  |
| 23  | DB    | 1                   | 41                  |
| 47  | D0    | 0                   | 1                   |
| All | All   | 1                   | 113                 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 23  | BB    | 1086 | A    | C5-C6 | -7.68 | 1.25        | 1.41     |
| 23  | DB    | 1086 | A    | C5-C6 | -7.66 | 1.25        | 1.41     |
| 52  | DI    | 3    | LYS  | CA-C  | 5.67  | 1.58        | 1.53     |
| 20  | AB    | 46   | VAL  | CA-CB | 5.27  | 1.56        | 1.54     |

All (260) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 42  | DU    | 49   | PRO  | N-CA-C      | -11.92 | 98.96       | 113.86   |
| 37  | DP    | 70   | GLU  | N-CA-C      | 10.38  | 124.67      | 108.79   |
| 23  | DB    | 2790 | U    | OP2-P-O3'   | 10.08  | 138.25      | 108.00   |
| 23  | BB    | 2790 | U    | OP1-P-O3'   | 10.00  | 138.01      | 108.00   |
| 27  | BE    | 74   | LYS  | N-CA-C      | -9.83  | 100.55      | 112.54   |
| 37  | BP    | 70   | GLU  | N-CA-C      | 9.78   | 123.22      | 108.46   |
| 33  | DL    | 118  | THR  | N-CA-C      | 9.71   | 131.26      | 109.81   |
| 37  | BP    | 79   | VAL  | N-CA-C      | 9.68   | 129.46      | 109.34   |
| 37  | DP    | 72   | VAL  | N-CA-C      | 9.66   | 129.43      | 109.34   |
| 23  | DB    | 2791 | G    | O5'-P-OP2   | -9.56  | 79.33       | 108.00   |
| 23  | BB    | 2791 | G    | O5'-P-OP1   | -9.54  | 79.37       | 108.00   |
| 37  | BP    | 71   | ARG  | N-CA-C      | 9.30   | 130.61      | 110.80   |
| 37  | BP    | 72   | VAL  | N-CA-C      | 9.16   | 128.39      | 109.34   |
| 23  | DB    | 2076 | U    | C2'-C3'-O3' | 9.10   | 127.35      | 113.70   |
| 37  | DP    | 71   | ARG  | N-CA-C      | 9.00   | 129.96      | 110.80   |
| 26  | BD    | 144  | GLY  | N-CA-C      | -8.87  | 103.39      | 114.92   |
| 28  | BF    | 106  | ALA  | N-CA-C      | 8.76   | 123.33      | 112.47   |
| 39  | BR    | 44   | GLY  | N-CA-C      | -8.70  | 102.41      | 114.67   |
| 23  | DB    | 2791 | G    | O5'-P-OP1   | 8.67   | 134.01      | 108.00   |
| 41  | DT    | 94   | ASP  | N-CA-C      | -8.62  | 101.21      | 112.24   |
| 1   | CA    | 328  | C    | C2'-C3'-O3' | 8.55   | 122.33      | 109.50   |
| 23  | BB    | 2791 | G    | O5'-P-OP2   | 8.54   | 133.63      | 108.00   |
| 1   | AA    | 328  | C    | C2'-C3'-O3' | 8.52   | 122.28      | 109.50   |
| 23  | DB    | 2790 | U    | O3'-P-O5'   | -8.52  | 91.22       | 104.00   |
| 37  | BP    | 40   | GLN  | N-CA-C      | -8.37  | 102.88      | 113.43   |
| 33  | DL    | 19   | LEU  | N-CA-C      | -8.12  | 102.33      | 112.72   |
| 33  | BL    | 6    | LEU  | N-CA-C      | 8.06   | 123.07      | 113.23   |
| 46  | BZ    | 41   | HIS  | CA-C-N      | 8.06   | 129.91      | 119.84   |
| 46  | BZ    | 41   | HIS  | C-N-CA      | 8.06   | 129.91      | 119.84   |
| 23  | BB    | 2790 | U    | O3'-P-O5'   | -8.06  | 91.92       | 104.00   |
| 32  | DK    | 80   | ASP  | N-CA-C      | -8.00  | 103.24      | 113.16   |
| 37  | BP    | 6    | GLN  | N-CA-C      | -7.99  | 103.65      | 113.15   |
| 39  | BR    | 40   | MET  | N-CA-C      | -7.88  | 103.39      | 113.16   |
| 28  | DF    | 14   | LYS  | N-CA-C      | -7.85  | 103.31      | 113.12   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 37  | DP    | 6    | GLN  | N-CA-C      | -7.80 | 103.02      | 112.54   |
| 1   | CA    | 1534 | A    | C2'-C3'-O3' | -7.77 | 97.84       | 109.50   |
| 33  | BL    | 28   | GLY  | N-CA-C      | -7.72 | 105.21      | 115.40   |
| 28  | BF    | 50   | ASP  | N-CA-C      | -7.69 | 102.83      | 112.90   |
| 46  | BZ    | 43   | PHE  | N-CA-C      | -7.68 | 97.74       | 109.95   |
| 39  | DR    | 39   | LEU  | N-CA-C      | -7.62 | 103.05      | 111.36   |
| 1   | CA    | 372  | C    | C2'-C3'-O3' | 7.58  | 120.87      | 109.50   |
| 1   | AA    | 372  | C    | C2'-C3'-O3' | 7.54  | 120.81      | 109.50   |
| 28  | DF    | 113  | PHE  | N-CA-C      | -7.46 | 97.53       | 109.76   |
| 37  | BP    | 14   | GLN  | N-CA-C      | -7.45 | 103.27      | 112.88   |
| 46  | DZ    | 55   | GLY  | N-CA-C      | -7.34 | 103.60      | 112.49   |
| 37  | DP    | 78   | PRO  | N-CA-C      | 7.31  | 122.02      | 111.13   |
| 43  | DW    | 43   | LYS  | N-CA-C      | -7.30 | 104.53      | 113.50   |
| 33  | DL    | 125  | LEU  | N-CA-C      | 7.21  | 119.28      | 107.23   |
| 44  | DX    | 54   | LYS  | N-CA-C      | -7.20 | 103.47      | 111.82   |
| 33  | DL    | 117  | THR  | N-CA-C      | -7.17 | 92.92       | 107.41   |
| 14  | CO    | 43   | ALA  | N-CA-C      | -7.06 | 103.59      | 111.71   |
| 29  | BG    | 158  | GLY  | N-CA-C      | -7.01 | 105.65      | 115.32   |
| 37  | DP    | 79   | VAL  | N-CA-C      | 7.01  | 123.92      | 109.34   |
| 39  | BR    | 51   | VAL  | N-CA-C      | 6.98  | 116.57      | 108.96   |
| 23  | DB    | 2790 | U    | C2'-C3'-O3' | -6.95 | 103.28      | 113.70   |
| 34  | BM    | 25   | ASP  | N-CA-C      | 6.89  | 118.25      | 108.74   |
| 34  | DM    | 132  | THR  | N-CA-C      | -6.89 | 102.88      | 112.25   |
| 33  | BL    | 18   | ARG  | N-CA-C      | 6.89  | 117.68      | 108.38   |
| 31  | DJ    | 3    | THR  | N-CA-C      | 6.88  | 120.52      | 108.75   |
| 37  | BP    | 95   | LYS  | N-CA-C      | -6.85 | 105.70      | 112.97   |
| 28  | DF    | 47   | LYS  | N-CA-C      | -6.80 | 104.85      | 113.01   |
| 34  | BM    | 100  | LYS  | N-CA-C      | 6.74  | 118.49      | 107.23   |
| 25  | DC    | 251  | THR  | CB-CA-C     | -6.73 | 108.83      | 116.63   |
| 26  | DD    | 97   | SER  | N-CA-C      | -6.72 | 104.94      | 113.01   |
| 39  | BR    | 53   | PHE  | N-CA-C      | 6.72  | 119.93      | 109.52   |
| 31  | DJ    | 5    | THR  | N-CA-C      | -6.67 | 98.38       | 108.52   |
| 32  | BK    | 16   | ALA  | N-CA-C      | 6.60  | 118.84      | 110.33   |
| 33  | BL    | 59   | ARG  | N-CA-C      | -6.56 | 103.53      | 113.89   |
| 33  | BL    | 76   | GLU  | N-CA-C      | -6.55 | 100.73      | 110.23   |
| 33  | BL    | 118  | THR  | CA-C-N      | 6.53  | 128.00      | 119.84   |
| 33  | BL    | 118  | THR  | C-N-CA      | 6.53  | 128.00      | 119.84   |
| 25  | DC    | 83   | ASP  | CA-C-N      | 6.53  | 126.55      | 119.89   |
| 25  | DC    | 83   | ASP  | C-N-CA      | 6.53  | 126.55      | 119.89   |
| 39  | BR    | 43   | ASN  | N-CA-C      | -6.50 | 104.53      | 113.56   |
| 25  | BC    | 124  | LYS  | CA-C-N      | -6.49 | 111.72      | 119.84   |
| 25  | BC    | 124  | LYS  | C-N-CA      | -6.49 | 111.72      | 119.84   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | DB    | 2076 | U    | C4'-C3'-O3' | 6.47  | 122.71      | 113.00   |
| 28  | BF    | 164  | GLU  | N-CA-C      | -6.47 | 104.27      | 111.71   |
| 1   | CA    | 1065 | U    | C2'-C3'-O3' | 6.44  | 119.15      | 109.50   |
| 34  | BM    | 68   | PHE  | CA-C-N      | 6.43  | 127.88      | 119.84   |
| 34  | BM    | 68   | PHE  | C-N-CA      | 6.43  | 127.88      | 119.84   |
| 40  | DS    | 47   | VAL  | N-CA-C      | -6.43 | 104.48      | 110.53   |
| 29  | DG    | 172  | GLU  | N-CA-C      | -6.43 | 99.73       | 109.95   |
| 28  | BF    | 107  | VAL  | N-CA-C      | -6.42 | 103.31      | 112.61   |
| 34  | DM    | 131  | VAL  | N-CA-C      | 6.41  | 116.27      | 108.06   |
| 20  | AB    | 44   | LYS  | N-CA-C      | -6.41 | 105.10      | 113.17   |
| 37  | DP    | 49   | ILE  | N-CA-C      | 6.37  | 122.58      | 109.34   |
| 34  | BM    | 132  | THR  | N-CA-C      | 6.36  | 124.34      | 110.80   |
| 32  | DK    | 15   | GLY  | N-CA-C      | -6.31 | 105.64      | 115.67   |
| 23  | DB    | 2336 | A    | C2'-C3'-O3' | 6.30  | 118.95      | 109.50   |
| 28  | BF    | 51   | ASN  | N-CA-C      | -6.30 | 105.35      | 113.16   |
| 23  | BB    | 2336 | A    | C2'-C3'-O3' | 6.28  | 118.92      | 109.50   |
| 39  | DR    | 29   | THR  | CB-CA-C     | -6.27 | 108.33      | 115.79   |
| 25  | BC    | 152  | GLN  | CB-CA-C     | -6.26 | 109.36      | 116.63   |
| 28  | DF    | 15   | LEU  | N-CA-C      | -6.26 | 105.60      | 113.18   |
| 37  | DP    | 50   | ARG  | N-CA-C      | -6.26 | 98.87       | 108.76   |
| 33  | BL    | 105  | ILE  | N-CA-C      | 6.25  | 116.86      | 110.05   |
| 28  | DF    | 50   | ASP  | N-CA-C      | -6.24 | 104.73      | 112.90   |
| 26  | DD    | 16   | THR  | N-CA-C      | -6.23 | 104.90      | 113.56   |
| 1   | AA    | 438  | U    | N1-C1'-C2'  | -6.22 | 104.66      | 114.00   |
| 27  | BE    | 45   | ALA  | N-CA-C      | -6.22 | 103.69      | 111.90   |
| 1   | CA    | 438  | U    | N1-C1'-C2'  | -6.21 | 104.69      | 114.00   |
| 40  | DS    | 30   | SER  | N-CA-C      | -6.18 | 104.54      | 111.28   |
| 34  | DM    | 6    | ARG  | N-CA-C      | -6.14 | 98.92       | 108.00   |
| 1   | CA    | 1201 | A    | C2'-C3'-O3' | 6.13  | 118.70      | 109.50   |
| 33  | DL    | 4    | ASN  | CB-CA-C     | -6.13 | 109.49      | 116.54   |
| 1   | AA    | 1528 | U    | C2'-C3'-O3' | 6.12  | 118.68      | 109.50   |
| 37  | BP    | 49   | ILE  | N-CA-C      | 6.11  | 122.05      | 109.34   |
| 28  | DF    | 74   | ALA  | N-CA-C      | 6.10  | 119.46      | 109.76   |
| 25  | DC    | 264  | LYS  | N-CA-C      | 6.08  | 115.88      | 107.73   |
| 1   | AA    | 960  | U    | C2'-C3'-O3' | 6.05  | 118.58      | 109.50   |
| 10  | CK    | 125  | LYS  | CB-CA-C     | -6.05 | 109.61      | 116.63   |
| 33  | DL    | 18   | ARG  | N-CA-C      | 6.02  | 118.54      | 108.96   |
| 27  | BE    | 107  | SER  | N-CA-C      | -6.00 | 105.66      | 112.87   |
| 23  | BB    | 1552 | A    | N9-C1'-C2'  | -6.00 | 103.00      | 112.00   |
| 46  | DZ    | 9    | TYR  | N-CA-C      | 6.00  | 116.47      | 108.38   |
| 52  | BI    | 63   | ASP  | N-CA-C      | -5.97 | 106.35      | 113.21   |
| 23  | DB    | 1552 | A    | N9-C1'-C2'  | -5.95 | 103.07      | 112.00   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 27  | DE    | 152  | GLU  | CB-CA-C     | -5.93 | 108.73      | 115.79   |
| 32  | DK    | 107  | LEU  | N-CA-C      | -5.91 | 106.02      | 113.18   |
| 2   | AC    | 137  | VAL  | N-CA-C      | -5.91 | 108.10      | 113.71   |
| 46  | DZ    | 52   | ALA  | N-CA-C      | -5.90 | 104.75      | 111.07   |
| 42  | DU    | 48   | VAL  | N-CA-C      | 5.85  | 121.52      | 108.88   |
| 34  | BM    | 24   | THR  | N-CA-C      | 5.85  | 117.31      | 110.41   |
| 35  | DN    | 81   | ASN  | N-CA-C      | 5.82  | 117.31      | 110.97   |
| 1   | AA    | 1065 | U    | C2'-C3'-O3' | 5.80  | 118.20      | 109.50   |
| 27  | BE    | 159  | LEU  | N-CA-C      | -5.79 | 106.26      | 113.15   |
| 35  | BN    | 2    | ARG  | N-CA-C      | -5.76 | 104.91      | 111.07   |
| 33  | DL    | 92   | LEU  | N-CA-C      | 5.73  | 123.01      | 110.80   |
| 43  | BW    | 17   | ALA  | N-CA-C      | 5.72  | 117.97      | 111.11   |
| 21  | AU    | 46   | ARG  | N-CA-C      | -5.71 | 106.45      | 113.41   |
| 46  | BZ    | 42   | PRO  | N-CA-C      | 5.71  | 124.23      | 112.47   |
| 27  | DE    | 159  | LEU  | N-CA-C      | -5.70 | 106.25      | 113.43   |
| 28  | BF    | 105  | ILE  | N-CA-C      | 5.69  | 116.96      | 108.54   |
| 28  | BF    | 143  | ASP  | N-CA-C      | -5.69 | 105.24      | 113.21   |
| 27  | BE    | 46   | GLN  | N-CA-C      | 5.69  | 117.96      | 111.02   |
| 50  | B3    | 34   | LYS  | N-CA-C      | -5.68 | 106.33      | 113.20   |
| 34  | DM    | 59   | ARG  | N-CA-C      | -5.68 | 106.57      | 112.93   |
| 33  | DL    | 6    | LEU  | N-CA-C      | -5.66 | 103.89      | 112.04   |
| 32  | DK    | 106  | GLU  | N-CA-C      | -5.66 | 105.49      | 112.90   |
| 23  | DB    | 727  | A    | N9-C1'-C2'  | 5.65  | 120.48      | 112.00   |
| 1   | CA    | 765  | G    | N9-C1'-C2'  | -5.65 | 103.53      | 112.00   |
| 23  | BB    | 1237 | A    | N9-C1'-C2'  | 5.64  | 120.46      | 112.00   |
| 11  | AL    | 101  | LEU  | CB-CA-C     | -5.63 | 110.06      | 116.54   |
| 1   | AA    | 765  | G    | N9-C1'-C2'  | -5.62 | 103.57      | 112.00   |
| 41  | DT    | 10   | VAL  | N-CA-C      | -5.62 | 106.31      | 113.22   |
| 30  | DH    | 27   | ARG  | N-CA-C      | -5.62 | 105.50      | 112.47   |
| 1   | CA    | 1319 | A    | N9-C1'-C2'  | 5.59  | 120.39      | 112.00   |
| 33  | DL    | 137  | ALA  | N-CA-C      | -5.59 | 106.25      | 112.57   |
| 47  | B0    | 37   | HIS  | CB-CA-C     | -5.59 | 110.15      | 116.63   |
| 30  | BH    | 37   | VAL  | N-CA-C      | 5.56  | 120.89      | 108.88   |
| 11  | CL    | 9    | LYS  | CA-C-N      | 5.55  | 126.77      | 119.84   |
| 11  | CL    | 9    | LYS  | C-N-CA      | 5.55  | 126.77      | 119.84   |
| 23  | DB    | 2430 | A    | N9-C1'-C2'  | 5.54  | 120.31      | 112.00   |
| 1   | CA    | 1009 | U    | N1-C1'-C2'  | 5.54  | 120.30      | 112.00   |
| 37  | BP    | 78   | PRO  | N-CA-C      | 5.53  | 123.87      | 112.47   |
| 1   | AA    | 1319 | A    | N9-C1'-C2'  | 5.53  | 120.30      | 112.00   |
| 32  | DK    | 9    | ASN  | CA-C-O      | 5.53  | 121.15      | 117.94   |
| 33  | BL    | 103  | ILE  | N-CA-C      | 5.53  | 116.21      | 109.30   |
| 30  | BH    | 124  | THR  | CB-CA-C     | -5.52 | 109.12      | 117.07   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | DB    | 299  | A    | N9-C1'-C2'  | 5.52  | 120.28      | 112.00   |
| 31  | DJ    | 102  | GLU  | N-CA-C      | -5.52 | 105.42      | 111.82   |
| 33  | BL    | 5    | THR  | N-CA-C      | -5.51 | 106.40      | 113.02   |
| 47  | B0    | 48   | TYR  | N-CA-C      | -5.49 | 106.75      | 113.50   |
| 1   | AA    | 1226 | C    | C2'-C3'-O3' | 5.48  | 117.73      | 109.50   |
| 23  | BB    | 2430 | A    | N9-C1'-C2'  | 5.48  | 120.22      | 112.00   |
| 1   | CA    | 1362 | A    | N9-C1'-C2'  | 5.48  | 120.21      | 112.00   |
| 1   | AA    | 576  | C    | C5'-C4'-C3' | 5.47  | 123.41      | 115.20   |
| 1   | AA    | 1049 | U    | C2'-C3'-O3' | 5.47  | 117.71      | 109.50   |
| 23  | BB    | 2733 | A    | N9-C1'-C2'  | -5.47 | 103.79      | 112.00   |
| 1   | CA    | 1432 | G    | N9-C1'-C2'  | -5.47 | 105.79      | 114.00   |
| 1   | CA    | 366  | A    | C2'-C3'-O3' | 5.47  | 117.70      | 109.50   |
| 23  | DB    | 544  | C    | C4'-C3'-O3' | 5.47  | 117.60      | 109.40   |
| 23  | DB    | 2733 | A    | N9-C1'-C2'  | -5.46 | 103.81      | 112.00   |
| 37  | DP    | 95   | LYS  | N-CA-C      | -5.46 | 106.59      | 113.20   |
| 1   | AA    | 366  | A    | C2'-C3'-O3' | 5.46  | 117.69      | 109.50   |
| 3   | AD    | 49   | ASP  | N-CA-C      | -5.46 | 107.63      | 114.56   |
| 1   | CA    | 437  | U    | N1-C1'-C2'  | 5.45  | 120.18      | 112.00   |
| 32  | DK    | 76   | VAL  | N-CA-C      | 5.45  | 115.10      | 106.32   |
| 23  | DB    | 1240 | U    | N1-C1'-C2'  | 5.45  | 120.17      | 112.00   |
| 20  | CB    | 16   | GLY  | N-CA-C      | 5.44  | 118.31      | 112.33   |
| 32  | DK    | 9    | ASN  | CB-CA-C     | -5.43 | 109.25      | 117.07   |
| 23  | BB    | 2103 | C    | N1-C1'-C2'  | 5.42  | 120.13      | 112.00   |
| 1   | AA    | 437  | U    | N1-C1'-C2'  | 5.42  | 120.13      | 112.00   |
| 7   | AH    | 66   | GLN  | CB-CA-C     | -5.42 | 109.27      | 117.07   |
| 42  | DU    | 50   | ALA  | N-CA-C      | -5.40 | 99.30       | 110.80   |
| 26  | DD    | 90   | PHE  | N-CA-C      | -5.40 | 99.30       | 110.80   |
| 33  | DL    | 41   | ARG  | N-CA-C      | -5.40 | 106.54      | 113.02   |
| 28  | DF    | 73   | VAL  | N-CA-C      | 5.40  | 120.56      | 109.34   |
| 33  | DL    | 116  | VAL  | N-CA-C      | 5.39  | 120.55      | 109.34   |
| 46  | BZ    | 60   | PHE  | N-CA-C      | -5.38 | 99.34       | 110.80   |
| 23  | DB    | 1419 | A    | N9-C1'-C2'  | 5.38  | 120.06      | 112.00   |
| 23  | BB    | 1419 | A    | N9-C1'-C2'  | 5.36  | 120.04      | 112.00   |
| 21  | CU    | 31   | VAL  | N-CA-C      | 5.36  | 111.94      | 106.21   |
| 26  | DD    | 102  | ALA  | CB-CA-C     | -5.36 | 110.38      | 116.54   |
| 27  | DE    | 147  | LEU  | N-CA-C      | 5.36  | 122.21      | 110.80   |
| 25  | BC    | 37   | SER  | CB-CA-C     | -5.34 | 109.38      | 117.07   |
| 36  | BO    | 58   | ILE  | N-CA-C      | -5.34 | 107.22      | 111.81   |
| 49  | B2    | 18   | PHE  | CB-CA-C     | -5.33 | 109.98      | 117.23   |
| 37  | DP    | 70   | GLU  | CA-C-N      | 5.33  | 131.73      | 121.54   |
| 37  | DP    | 70   | GLU  | C-N-CA      | 5.33  | 131.73      | 121.54   |
| 33  | BL    | 26   | GLY  | N-CA-C      | -5.33 | 107.27      | 116.01   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 43  | BW    | 3    | LYS  | N-CA-C      | -5.33 | 105.05      | 112.30   |
| 23  | DB    | 1237 | A    | N9-C1'-C2'  | 5.33  | 119.99      | 112.00   |
| 39  | DR    | 61   | ALA  | N-CA-C      | -5.32 | 105.60      | 112.68   |
| 27  | BE    | 50   | ALA  | N-CA-C      | -5.30 | 106.78      | 113.20   |
| 1   | CA    | 1225 | A    | N9-C1'-C2'  | 5.30  | 119.95      | 112.00   |
| 1   | CA    | 1030 | U    | C2'-C3'-O3' | 5.30  | 117.45      | 109.50   |
| 21  | CU    | 24   | LYS  | CB-CA-C     | -5.30 | 110.44      | 116.54   |
| 32  | BK    | 13   | ASN  | N-CA-C      | 5.29  | 115.52      | 108.38   |
| 36  | DO    | 21   | LEU  | CB-CA-C     | -5.29 | 110.50      | 116.63   |
| 10  | CK    | 124  | LYS  | N-CA-C      | -5.29 | 105.41      | 111.07   |
| 1   | CA    | 1285 | A    | N9-C1'-C2'  | 5.29  | 119.93      | 112.00   |
| 1   | CA    | 1226 | C    | C2'-C3'-O3' | 5.28  | 117.42      | 109.50   |
| 47  | D0    | 22   | THR  | CB-CA-C     | -5.26 | 108.80      | 116.53   |
| 41  | BT    | 94   | ASP  | CB-CA-C     | -5.24 | 109.55      | 115.79   |
| 42  | DU    | 74   | ALA  | N-CA-C      | 5.24  | 113.08      | 108.78   |
| 38  | BQ    | 107  | ALA  | N-CA-C      | -5.24 | 106.89      | 113.28   |
| 39  | DR    | 46   | GLU  | CB-CA-C     | -5.23 | 109.57      | 115.79   |
| 26  | BD    | 154  | LYS  | N-CA-C      | -5.22 | 99.67       | 110.80   |
| 25  | BC    | 264  | LYS  | N-CA-C      | 5.22  | 116.59      | 109.18   |
| 14  | AO    | 43   | ALA  | N-CA-C      | -5.21 | 105.71      | 111.71   |
| 25  | BC    | 83   | ASP  | CA-C-N      | 5.21  | 126.36      | 119.84   |
| 25  | BC    | 83   | ASP  | C-N-CA      | 5.21  | 126.36      | 119.84   |
| 6   | CG    | 146  | ALA  | N-CA-C      | -5.21 | 106.61      | 113.17   |
| 52  | BI    | 65   | SER  | N-CA-C      | -5.21 | 103.16      | 110.35   |
| 28  | DF    | 19   | PHE  | N-CA-C      | -5.21 | 105.81      | 113.72   |
| 32  | DK    | 89   | ASN  | N-CA-C      | 5.20  | 121.88      | 110.80   |
| 36  | BO    | 6    | ALA  | N-CA-C      | -5.19 | 106.75      | 114.64   |
| 1   | AA    | 1009 | U    | N1-C1'-C2'  | 5.18  | 119.77      | 112.00   |
| 33  | BL    | 122  | VAL  | N-CA-C      | 5.17  | 116.68      | 109.55   |
| 34  | BM    | 66   | ARG  | N-CA-C      | 5.16  | 117.51      | 107.71   |
| 36  | DO    | 16   | ARG  | N-CA-C      | -5.16 | 106.94      | 113.18   |
| 5   | AF    | 18   | VAL  | CB-CA-C     | -5.16 | 108.80      | 113.70   |
| 23  | BB    | 1250 | G    | C2'-C3'-O3' | 5.16  | 117.23      | 109.50   |
| 37  | BP    | 33   | GLU  | CB-CA-C     | -5.15 | 110.22      | 117.23   |
| 1   | CA    | 1400 | C    | N1-C1'-C2'  | 5.15  | 119.73      | 112.00   |
| 23  | BB    | 299  | A    | N9-C1'-C2'  | 5.14  | 119.72      | 112.00   |
| 41  | BT    | 76   | ARG  | N-CA-C      | 5.14  | 115.07      | 108.34   |
| 28  | BF    | 47   | LYS  | N-CA-C      | -5.13 | 105.69      | 111.28   |
| 43  | DW    | 11   | ASN  | N-CA-C      | -5.12 | 106.53      | 112.89   |
| 52  | BI    | 66   | PHE  | N-CA-C      | 5.12  | 116.07      | 108.60   |
| 36  | BO    | 91   | SER  | CB-CA-C     | -5.10 | 109.72      | 117.07   |
| 36  | BO    | 16   | ARG  | N-CA-C      | -5.09 | 107.02      | 113.18   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | DN    | 63   | ARG  | N-CA-C      | -5.09 | 106.17      | 112.38   |
| 46  | DZ    | 61   | ASN  | N-CA-C      | -5.09 | 107.14      | 113.55   |
| 26  | DD    | 151  | THR  | CA-C-N      | 5.07  | 126.17      | 119.84   |
| 26  | DD    | 151  | THR  | C-N-CA      | 5.07  | 126.17      | 119.84   |
| 41  | DT    | 64   | LYS  | CB-CA-C     | -5.07 | 109.77      | 117.07   |
| 52  | DI    | 3    | LYS  | CA-C-N      | 5.07  | 129.88      | 122.69   |
| 52  | DI    | 3    | LYS  | C-N-CA      | 5.07  | 129.88      | 122.69   |
| 26  | BD    | 201  | LEU  | CB-CA-C     | -5.06 | 109.77      | 115.79   |
| 32  | DK    | 77   | ILE  | N-CA-C      | -5.04 | 102.35      | 109.21   |
| 42  | DU    | 41   | VAL  | N-CA-C      | 5.04  | 115.29      | 107.78   |
| 23  | DB    | 125  | A    | C2'-C3'-O3' | 5.04  | 117.06      | 109.50   |
| 46  | BZ    | 59   | ARG  | O-C-N       | 5.04  | 124.56      | 120.83   |
| 41  | DT    | 28   | ASN  | N-CA-C      | -5.04 | 107.08      | 113.23   |
| 32  | BK    | 74   | GLY  | N-CA-C      | -5.02 | 108.51      | 114.48   |
| 36  | BO    | 91   | SER  | CA-C-O      | 5.01  | 120.85      | 117.94   |
| 23  | DB    | 1439 | A    | N9-C1'-C2'  | -5.01 | 104.49      | 112.00   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 23  | DB    | 2076 | U    | C3'  |

All (113) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | AA    | 1047 | G    | Sidechain |
| 1   | AA    | 1319 | A    | Sidechain |
| 1   | AA    | 1331 | G    | Sidechain |
| 1   | AA    | 1441 | A    | Sidechain |
| 1   | AA    | 187  | G    | Sidechain |
| 1   | AA    | 281  | G    | Sidechain |
| 1   | AA    | 324  | G    | Sidechain |
| 1   | AA    | 437  | U    | Sidechain |
| 1   | AA    | 438  | U    | Sidechain |
| 1   | AA    | 454  | G    | Sidechain |
| 1   | AA    | 496  | A    | Sidechain |
| 1   | AA    | 521  | G    | Sidechain |
| 1   | AA    | 575  | G    | Sidechain |
| 1   | AA    | 703  | G    | Sidechain |
| 23  | BB    | 1047 | G    | Sidechain |
| 23  | BB    | 1060 | U    | Sidechain |
| 23  | BB    | 1086 | A    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 23  | BB    | 1088 | A    | Sidechain |
| 23  | BB    | 1119 | U    | Sidechain |
| 23  | BB    | 1240 | U    | Sidechain |
| 23  | BB    | 1250 | G    | Sidechain |
| 23  | BB    | 1419 | A    | Sidechain |
| 23  | BB    | 1439 | A    | Sidechain |
| 23  | BB    | 1450 | G    | Sidechain |
| 23  | BB    | 1462 | C    | Sidechain |
| 23  | BB    | 1546 | G    | Sidechain |
| 23  | BB    | 1572 | A    | Sidechain |
| 23  | BB    | 1828 | G    | Sidechain |
| 23  | BB    | 2108 | A    | Sidechain |
| 23  | BB    | 221  | A    | Sidechain |
| 23  | BB    | 2213 | U    | Sidechain |
| 23  | BB    | 222  | A    | Sidechain |
| 23  | BB    | 2267 | A    | Sidechain |
| 23  | BB    | 2272 | U    | Sidechain |
| 23  | BB    | 2318 | G    | Sidechain |
| 23  | BB    | 2413 | G    | Sidechain |
| 23  | BB    | 2471 | A    | Sidechain |
| 23  | BB    | 2638 | G    | Sidechain |
| 23  | BB    | 2733 | A    | Sidechain |
| 23  | BB    | 2770 | G    | Sidechain |
| 23  | BB    | 2834 | G    | Sidechain |
| 23  | BB    | 2848 | G    | Sidechain |
| 23  | BB    | 2857 | G    | Sidechain |
| 23  | BB    | 2868 | A    | Sidechain |
| 23  | BB    | 2883 | A    | Sidechain |
| 23  | BB    | 299  | A    | Sidechain |
| 23  | BB    | 361  | G    | Sidechain |
| 23  | BB    | 500  | G    | Sidechain |
| 23  | BB    | 51   | G    | Sidechain |
| 23  | BB    | 630  | G    | Sidechain |
| 23  | BB    | 633  | A    | Sidechain |
| 23  | BB    | 727  | A    | Sidechain |
| 23  | BB    | 729  | G    | Sidechain |
| 23  | BB    | 757  | G    | Sidechain |
| 23  | BB    | 942  | G    | Sidechain |
| 1   | CA    | 1133 | G    | Sidechain |
| 1   | CA    | 1319 | A    | Sidechain |
| 1   | CA    | 1362 | A    | Sidechain |
| 1   | CA    | 1432 | G    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | CA    | 1441 | A    | Sidechain |
| 1   | CA    | 187  | G    | Sidechain |
| 1   | CA    | 281  | G    | Sidechain |
| 1   | CA    | 324  | G    | Sidechain |
| 1   | CA    | 437  | U    | Sidechain |
| 1   | CA    | 438  | U    | Sidechain |
| 1   | CA    | 454  | G    | Sidechain |
| 1   | CA    | 496  | A    | Sidechain |
| 1   | CA    | 521  | G    | Sidechain |
| 1   | CA    | 575  | G    | Sidechain |
| 1   | CA    | 703  | G    | Sidechain |
| 1   | CA    | 83   | C    | Sidechain |
| 47  | D0    | 48   | TYR  | Sidechain |
| 23  | DB    | 1047 | G    | Sidechain |
| 23  | DB    | 1060 | U    | Sidechain |
| 23  | DB    | 1086 | A    | Sidechain |
| 23  | DB    | 1088 | A    | Sidechain |
| 23  | DB    | 1247 | A    | Sidechain |
| 23  | DB    | 136  | G    | Sidechain |
| 23  | DB    | 1419 | A    | Sidechain |
| 23  | DB    | 1439 | A    | Sidechain |
| 23  | DB    | 1450 | G    | Sidechain |
| 23  | DB    | 1462 | C    | Sidechain |
| 23  | DB    | 1546 | G    | Sidechain |
| 23  | DB    | 1572 | A    | Sidechain |
| 23  | DB    | 1828 | G    | Sidechain |
| 23  | DB    | 2062 | A    | Sidechain |
| 23  | DB    | 2108 | A    | Sidechain |
| 23  | DB    | 214  | G    | Sidechain |
| 23  | DB    | 221  | A    | Sidechain |
| 23  | DB    | 222  | A    | Sidechain |
| 23  | DB    | 2267 | A    | Sidechain |
| 23  | DB    | 2272 | U    | Sidechain |
| 23  | DB    | 232  | G    | Sidechain |
| 23  | DB    | 2413 | G    | Sidechain |
| 23  | DB    | 2471 | A    | Sidechain |
| 23  | DB    | 2503 | A    | Sidechain |
| 23  | DB    | 2638 | G    | Sidechain |
| 23  | DB    | 2733 | A    | Sidechain |
| 23  | DB    | 2770 | G    | Sidechain |
| 23  | DB    | 28   | A    | Sidechain |
| 23  | DB    | 2834 | G    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 23  | DB    | 2848 | G    | Sidechain |
| 23  | DB    | 2857 | G    | Sidechain |
| 23  | DB    | 2868 | A    | Sidechain |
| 23  | DB    | 2883 | A    | Sidechain |
| 23  | DB    | 299  | A    | Sidechain |
| 23  | DB    | 500  | G    | Sidechain |
| 23  | DB    | 630  | G    | Sidechain |
| 23  | DB    | 633  | A    | Sidechain |
| 23  | DB    | 727  | A    | Sidechain |
| 23  | DB    | 729  | G    | Sidechain |
| 23  | DB    | 757  | G    | Sidechain |
| 23  | DB    | 858  | G    | Sidechain |

## 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   | AA    | 32831 | 0        | 16521    | 1328    | 0            |
| 1   | CA    | 32831 | 0        | 16521    | 1388    | 0            |
| 2   | AC    | 1624  | 0        | 1699     | 195     | 0            |
| 2   | CC    | 1624  | 0        | 1699     | 167     | 0            |
| 3   | AD    | 1643  | 0        | 1710     | 190     | 0            |
| 3   | CD    | 1643  | 0        | 1710     | 185     | 0            |
| 4   | AE    | 1105  | 0        | 1148     | 111     | 0            |
| 4   | CE    | 1105  | 0        | 1148     | 150     | 0            |
| 5   | AF    | 817   | 0        | 808      | 79      | 0            |
| 5   | CF    | 817   | 0        | 808      | 105     | 0            |
| 6   | AG    | 1174  | 0        | 1230     | 110     | 0            |
| 6   | CG    | 1196  | 0        | 1246     | 108     | 0            |
| 7   | AH    | 979   | 0        | 1034     | 88      | 0            |
| 7   | CH    | 979   | 0        | 1034     | 83      | 0            |
| 8   | AI    | 1022  | 0        | 1070     | 159     | 0            |
| 8   | CI    | 1022  | 0        | 1070     | 130     | 0            |
| 9   | AJ    | 786   | 0        | 828      | 97      | 0            |
| 9   | CJ    | 786   | 0        | 828      | 113     | 0            |
| 10  | AK    | 877   | 0        | 887      | 108     | 0            |
| 10  | CK    | 877   | 0        | 887      | 107     | 0            |
| 11  | AL    | 955   | 0        | 1019     | 106     | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 11  | CL    | 955   | 0        | 1019     | 92      | 0            |
| 12  | AM    | 883   | 0        | 944      | 92      | 0            |
| 12  | CM    | 876   | 0        | 937      | 117     | 0            |
| 13  | AN    | 774   | 0        | 827      | 113     | 0            |
| 13  | CN    | 774   | 0        | 827      | 126     | 0            |
| 14  | AO    | 716   | 0        | 742      | 56      | 0            |
| 14  | CO    | 716   | 0        | 742      | 58      | 0            |
| 15  | AP    | 649   | 0        | 666      | 82      | 0            |
| 15  | CP    | 638   | 0        | 656      | 83      | 0            |
| 16  | AQ    | 648   | 0        | 691      | 104     | 0            |
| 16  | CQ    | 657   | 0        | 702      | 91      | 0            |
| 17  | AR    | 455   | 0        | 478      | 49      | 0            |
| 17  | CR    | 455   | 0        | 478      | 47      | 0            |
| 18  | AS    | 637   | 0        | 665      | 89      | 0            |
| 18  | CS    | 644   | 0        | 675      | 100     | 0            |
| 19  | AT    | 665   | 0        | 714      | 65      | 0            |
| 19  | CT    | 665   | 0        | 714      | 64      | 0            |
| 20  | AB    | 1704  | 0        | 1732     | 202     | 0            |
| 20  | CB    | 1704  | 0        | 1732     | 179     | 0            |
| 21  | AU    | 425   | 0        | 449      | 71      | 0            |
| 21  | CU    | 425   | 0        | 449      | 67      | 0            |
| 22  | BA    | 2507  | 0        | 1270     | 83      | 0            |
| 22  | DA    | 2507  | 0        | 1270     | 119     | 0            |
| 23  | BB    | 60995 | 0        | 30678    | 2748    | 0            |
| 23  | DB    | 60995 | 0        | 30677    | 2694    | 0            |
| 24  | BV    | 753   | 0        | 780      | 107     | 0            |
| 24  | DV    | 753   | 0        | 780      | 72      | 0            |
| 25  | BC    | 2053  | 0        | 2122     | 470     | 0            |
| 25  | DC    | 2053  | 0        | 2122     | 396     | 0            |
| 26  | BD    | 1565  | 0        | 1616     | 387     | 0            |
| 26  | DD    | 1565  | 0        | 1616     | 323     | 0            |
| 27  | BE    | 1552  | 0        | 1619     | 293     | 0            |
| 27  | DE    | 1552  | 0        | 1619     | 274     | 0            |
| 28  | BF    | 1420  | 0        | 1460     | 180     | 0            |
| 28  | DF    | 1420  | 0        | 1460     | 166     | 0            |
| 29  | BG    | 1323  | 0        | 1374     | 168     | 0            |
| 29  | DG    | 1323  | 0        | 1374     | 168     | 0            |
| 30  | BH    | 1111  | 0        | 1148     | 178     | 0            |
| 30  | DH    | 1111  | 0        | 1148     | 172     | 0            |
| 31  | BJ    | 1112  | 0        | 1147     | 222     | 0            |
| 31  | DJ    | 1112  | 0        | 1147     | 217     | 0            |
| 32  | BK    | 930   | 0        | 1000     | 130     | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 32  | DK    | 930   | 0        | 1000     | 127     | 0            |
| 33  | BL    | 1053  | 0        | 1129     | 290     | 0            |
| 33  | DL    | 1053  | 0        | 1129     | 253     | 0            |
| 34  | BM    | 1074  | 0        | 1157     | 244     | 0            |
| 34  | DM    | 1074  | 0        | 1157     | 183     | 0            |
| 35  | BN    | 1008  | 0        | 1045     | 189     | 0            |
| 35  | DN    | 1008  | 0        | 1045     | 163     | 0            |
| 36  | BO    | 900   | 0        | 935      | 138     | 0            |
| 36  | DO    | 900   | 0        | 935      | 147     | 0            |
| 37  | BP    | 917   | 0        | 965      | 202     | 0            |
| 37  | DP    | 917   | 0        | 965      | 200     | 0            |
| 38  | BQ    | 947   | 0        | 1022     | 206     | 0            |
| 38  | DQ    | 947   | 0        | 1022     | 182     | 0            |
| 39  | BR    | 816   | 0        | 839      | 176     | 0            |
| 39  | DR    | 816   | 0        | 839      | 170     | 0            |
| 40  | BS    | 857   | 0        | 922      | 128     | 0            |
| 40  | DS    | 857   | 0        | 922      | 125     | 0            |
| 41  | BT    | 777   | 0        | 840      | 154     | 0            |
| 41  | DT    | 777   | 0        | 840      | 138     | 0            |
| 42  | BU    | 779   | 0        | 834      | 167     | 0            |
| 42  | DU    | 779   | 0        | 834      | 127     | 0            |
| 43  | BW    | 634   | 0        | 656      | 166     | 0            |
| 43  | DW    | 634   | 0        | 656      | 174     | 0            |
| 44  | BX    | 509   | 0        | 543      | 90      | 0            |
| 44  | DX    | 509   | 0        | 543      | 85      | 0            |
| 45  | BY    | 449   | 0        | 491      | 62      | 0            |
| 45  | DY    | 449   | 0        | 491      | 85      | 0            |
| 46  | BZ    | 549   | 0        | 552      | 120     | 0            |
| 46  | DZ    | 549   | 0        | 552      | 107     | 0            |
| 47  | B0    | 444   | 0        | 461      | 80      | 0            |
| 47  | D0    | 444   | 0        | 461      | 93      | 0            |
| 48  | B1    | 441   | 0        | 485      | 83      | 0            |
| 48  | D1    | 441   | 0        | 485      | 80      | 0            |
| 49  | B2    | 377   | 0        | 418      | 62      | 0            |
| 49  | D2    | 377   | 0        | 418      | 69      | 0            |
| 50  | B3    | 504   | 0        | 574      | 118     | 0            |
| 50  | D3    | 504   | 0        | 574      | 110     | 0            |
| 51  | B4    | 302   | 0        | 343      | 62      | 0            |
| 51  | D4    | 302   | 0        | 343      | 79      | 0            |
| 52  | BI    | 1032  | 0        | 1088     | 127     | 0            |
| 52  | DI    | 1032  | 0        | 1088     | 189     | 0            |
| 53  | AA    | 26    | 0        | 23       | 3       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 53  | CA    | 26     | 0        | 23       | 1       | 0            |
| 54  | AA    | 60     | 0        | 0        | 0       | 0            |
| 54  | BB    | 110    | 0        | 0        | 0       | 0            |
| 54  | CA    | 62     | 0        | 0        | 0       | 0            |
| 54  | DB    | 109    | 0        | 0        | 0       | 0            |
| 54  | DE    | 1      | 0        | 0        | 0       | 0            |
| 54  | DN    | 1      | 0        | 0        | 0       | 0            |
| 55  | AA    | 289    | 0        | 0        | 1       | 0            |
| 55  | AE    | 3      | 0        | 0        | 0       | 0            |
| 55  | AK    | 2      | 0        | 0        | 0       | 0            |
| 55  | AN    | 3      | 0        | 0        | 0       | 0            |
| 55  | AP    | 2      | 0        | 0        | 0       | 0            |
| 55  | AT    | 1      | 0        | 0        | 0       | 0            |
| 55  | BB    | 497    | 0        | 0        | 11      | 0            |
| 55  | BC    | 1      | 0        | 0        | 0       | 0            |
| 55  | BE    | 5      | 0        | 0        | 0       | 0            |
| 55  | BH    | 1      | 0        | 0        | 0       | 0            |
| 55  | BL    | 2      | 0        | 0        | 0       | 0            |
| 55  | BN    | 1      | 0        | 0        | 0       | 0            |
| 55  | CA    | 293    | 0        | 0        | 1       | 0            |
| 55  | CE    | 3      | 0        | 0        | 0       | 0            |
| 55  | CK    | 1      | 0        | 0        | 0       | 0            |
| 55  | CL    | 4      | 0        | 0        | 0       | 0            |
| 55  | CN    | 3      | 0        | 0        | 0       | 0            |
| 55  | CP    | 1      | 0        | 0        | 0       | 0            |
| 55  | CT    | 3      | 0        | 0        | 0       | 0            |
| 55  | D2    | 2      | 0        | 0        | 0       | 0            |
| 55  | DB    | 501    | 0        | 0        | 10      | 0            |
| 55  | DC    | 1      | 0        | 0        | 0       | 0            |
| 55  | DD    | 1      | 0        | 0        | 0       | 0            |
| 55  | DE    | 3      | 0        | 0        | 0       | 0            |
| 55  | DL    | 1      | 0        | 0        | 0       | 0            |
| 55  | DN    | 2      | 0        | 0        | 0       | 0            |
| 55  | DT    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 284160 | 0        | 190815   | 20206   | 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 43.

All (20206) 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) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:1099:G:O5'   | 52:DI:4:VAL:N      | 1.71                     | 1.23              |
| 32:DK:78:ARG:HG2   | 37:DP:72:VAL:HG21  | 1.24                     | 1.15              |
| 23:DB:1098:A:H3'   | 52:DI:3:LYS:CA     | 1.76                     | 1.15              |
| 23:DB:587:C:H3'    | 33:DL:29:LYS:HD2   | 1.20                     | 1.14              |
| 48:D1:29:LYS:HB2   | 48:D1:30:PRO:HD3   | 1.30                     | 1.14              |
| 1:AA:699:C:H2'     | 1:AA:700:G:H5''    | 1.28                     | 1.14              |
| 23:BB:662:G:H4'    | 33:BL:24:GLY:H     | 1.11                     | 1.13              |
| 42:DU:60:LYS:HE3   | 42:DU:61:GLU:H     | 1.08                     | 1.13              |
| 23:DB:458:G:H5''   | 49:D2:39:ARG:HB2   | 1.30                     | 1.12              |
| 44:DX:43:LEU:HB2   | 44:DX:45:GLN:HE22  | 1.13                     | 1.12              |
| 23:BB:85:G:H5'     | 42:BU:28:LEU:HA    | 1.30                     | 1.11              |
| 1:CA:243:A:H4'     | 1:CA:244:U:H5'     | 1.29                     | 1.11              |
| 20:AB:163:ILE:HG23 | 20:AB:164:ASP:H    | 1.14                     | 1.11              |
| 33:DL:7:SER:HB2    | 33:DL:8:PRO:HD3    | 1.24                     | 1.11              |
| 36:BO:57:ALA:HB2   | 36:BO:62:LEU:HD22  | 1.30                     | 1.10              |
| 32:BK:108:ARG:HH21 | 37:BP:36:LYS:HG3   | 1.06                     | 1.10              |
| 30:BH:82:SER:H     | 30:BH:146:VAL:HG13 | 1.16                     | 1.10              |
| 23:BB:2750:A:H4'   | 29:BG:1:SER:HB2    | 1.34                     | 1.09              |
| 34:BM:3:GLN:H      | 34:BM:4:PRO:HD2    | 1.04                     | 1.09              |
| 33:BL:14:LYS:HZ2   | 33:BL:14:LYS:HA    | 1.15                     | 1.09              |
| 34:DM:57:VAL:HG21  | 34:DM:112:LEU:HD21 | 1.33                     | 1.09              |
| 23:BB:38:A:O4'     | 27:BE:46:GLN:HG3   | 1.53                     | 1.08              |
| 20:CB:46:VAL:HG13  | 20:CB:47:PRO:HD3   | 1.35                     | 1.08              |
| 11:CL:43:LYS:HB3   | 11:CL:44:PRO:HD2   | 1.28                     | 1.08              |
| 25:DC:33:LEU:HD22  | 25:DC:34:GLU:HG3   | 1.35                     | 1.08              |
| 1:CA:974:A:H4'     | 1:CA:975:A:H5'     | 1.28                     | 1.08              |
| 1:CA:699:C:H2'     | 1:CA:700:G:H5''    | 1.28                     | 1.08              |
| 23:DB:2527:C:H5''  | 51:D4:34:LYS:HG3   | 1.35                     | 1.08              |
| 1:AA:243:A:H4'     | 1:AA:244:U:H5'     | 1.29                     | 1.07              |
| 26:BD:24:VAL:HG21  | 26:BD:193:VAL:HG11 | 1.36                     | 1.06              |
| 43:DW:38:ARG:HH21  | 43:DW:40:ARG:HD3   | 1.16                     | 1.06              |
| 25:BC:42:ARG:HG2   | 25:BC:43:ASN:H     | 1.14                     | 1.06              |
| 23:BB:100:U:H4'    | 42:BU:90:LYS:HE2   | 1.36                     | 1.05              |
| 23:DB:1098:A:H3'   | 52:DI:3:LYS:HA     | 1.37                     | 1.05              |
| 23:BB:161:A:H3'    | 23:BB:162:U:H5''   | 1.35                     | 1.05              |
| 25:BC:107:LYS:HB2  | 25:BC:194:VAL:HG11 | 1.39                     | 1.05              |
| 23:BB:2204:G:H5'   | 25:BC:149:LYS:HE3  | 1.36                     | 1.04              |
| 23:DB:45:G:H5''    | 23:DB:46:G:H5'     | 1.36                     | 1.04              |
| 23:BB:2333:A:H4'   | 23:BB:2334:U:H5''  | 1.40                     | 1.04              |
| 23:DB:1099:G:H8    | 52:DI:3:LYS:N      | 1.56                     | 1.04              |
| 25:DC:107:LYS:HB2  | 25:DC:194:VAL:HG21 | 1.38                     | 1.04              |
| 30:DH:3:VAL:HG22   | 30:DH:21:VAL:HG11  | 1.39                     | 1.04              |

Continued on next page...

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:DN:45:ARG:HH22 | 35:DN:113:ILE:HG23 | 1.21                     | 1.04              |
| 31:BJ:135:GLN:HG2 | 31:BJ:137:PRO:HD2  | 1.40                     | 1.03              |
| 31:DJ:102:GLU:HG3 | 31:DJ:124:VAL:HG12 | 1.40                     | 1.03              |
| 43:BW:47:GLY:HA3  | 43:BW:55:ASP:HB3   | 1.39                     | 1.03              |
| 18:AS:18:VAL:HG21 | 18:AS:43:MET:HG2   | 1.35                     | 1.03              |
| 37:BP:52:ARG:HB3  | 37:BP:60:VAL:HG11  | 1.37                     | 1.03              |
| 36:DO:56:LYS:HE2  | 36:DO:81:ARG:HE    | 1.16                     | 1.03              |
| 38:DQ:48:ASP:HA   | 38:DQ:51:GLN:HE21  | 1.20                     | 1.03              |
| 20:AB:46:VAL:HG13 | 20:AB:47:PRO:HD3   | 1.38                     | 1.03              |
| 23:BB:923:G:H1'   | 43:BW:23:LYS:HD3   | 1.38                     | 1.03              |
| 27:BE:128:ALA:HB3 | 27:BE:129:PRO:HD3  | 1.36                     | 1.03              |
| 30:BH:37:VAL:H    | 30:BH:38:PRO:HD2   | 1.23                     | 1.03              |
| 42:DU:28:LEU:HD13 | 42:DU:30:SER:H     | 1.24                     | 1.03              |
| 23:DB:323:C:H1'   | 27:DE:164:LEU:HB3  | 1.39                     | 1.02              |
| 33:DL:51:GLU:HG2  | 33:DL:52:GLY:H     | 1.24                     | 1.02              |
| 51:D4:26:ILE:HG13 | 51:D4:35:GLN:H     | 1.22                     | 1.02              |
| 30:DH:6:LEU:HD12  | 30:DH:36:ALA:H     | 1.24                     | 1.02              |
| 33:BL:61:LEU:HB3  | 33:BL:62:PRO:HD2   | 1.42                     | 1.02              |
| 37:DP:93:LYS:HG2  | 37:DP:96:LEU:HA    | 1.41                     | 1.02              |
| 15:AP:42:ILE:HB   | 15:AP:46:LYS:HD2   | 1.42                     | 1.02              |
| 32:BK:71:ARG:HB3  | 32:BK:72:PRO:HD2   | 1.04                     | 1.02              |
| 45:BY:16:LEU:HB2  | 45:BY:17:PRO:HD3   | 1.37                     | 1.02              |
| 33:BL:13:LYS:HG3  | 33:BL:14:LYS:H     | 1.25                     | 1.02              |
| 46:BZ:8:LYS:HD2   | 46:BZ:9:TYR:H      | 1.22                     | 1.02              |
| 32:BK:71:ARG:HB3  | 32:BK:72:PRO:CD    | 1.90                     | 1.01              |
| 32:BK:8:LEU:HD23  | 32:BK:82:ASN:HB3   | 1.41                     | 1.01              |
| 23:DB:1099:G:P    | 52:DI:4:VAL:H      | 1.83                     | 1.01              |
| 37:DP:47:ILE:HG22 | 37:DP:48:ALA:H     | 1.22                     | 1.01              |
| 23:DB:2091:C:H3'  | 23:DB:2092:U:H5''  | 1.43                     | 1.01              |
| 8:CI:27:ILE:HG23  | 8:CI:34:LEU:HB2    | 1.42                     | 1.00              |
| 23:DB:2333:A:H4'  | 23:DB:2334:U:H5''  | 1.40                     | 1.00              |
| 48:D1:46:VAL:HG13 | 48:D1:47:ILE:HG13  | 1.41                     | 1.00              |
| 34:BM:38:ARG:HH11 | 34:BM:38:ARG:HB2   | 1.26                     | 1.00              |
| 23:BB:1454:C:H5'  | 35:BN:63:ARG:HH21  | 1.24                     | 1.00              |
| 23:BB:2052:A:H4'  | 26:BD:148:GLN:H    | 1.24                     | 1.00              |
| 23:DB:1025:G:H1'  | 23:DB:1135:C:H5'   | 1.43                     | 1.00              |
| 24:DV:63:ILE:H    | 24:DV:70:ILE:HD11  | 1.23                     | 1.00              |
| 23:BB:442:G:H1'   | 27:BE:44:ARG:HD2   | 1.38                     | 1.00              |
| 23:BB:692:C:H5'   | 25:BC:42:ARG:HB2   | 1.40                     | 1.00              |
| 16:AQ:76:ARG:HE   | 16:AQ:78:VAL:HG22  | 1.27                     | 1.00              |
| 11:AL:8:ARG:HG3   | 11:AL:9:LYS:H      | 1.24                     | 1.00              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:CF:3:HIS:HB3     | 5:CF:92:THR:HA     | 1.41                     | 1.00              |
| 23:DB:136:G:H2'    | 23:DB:137:U:C6     | 1.97                     | 0.99              |
| 20:AB:67:LEU:HD11  | 20:AB:157:PRO:HB3  | 1.44                     | 0.99              |
| 25:DC:107:LYS:HE3  | 25:DC:108:GLY:H    | 1.23                     | 0.99              |
| 26:DD:197:THR:HG23 | 26:DD:198:GLY:H    | 1.28                     | 0.99              |
| 46:DZ:55:GLY:HA2   | 46:DZ:59:ARG:HB2   | 1.43                     | 0.99              |
| 3:AD:7:LYS:HE2     | 3:AD:20:LEU:HD13   | 1.43                     | 0.99              |
| 25:DC:230:PRO:HG2  | 25:DC:245:THR:H    | 1.27                     | 0.99              |
| 25:DC:171:VAL:HB   | 25:DC:182:LYS:HB3  | 1.45                     | 0.99              |
| 1:CA:973:G:H3'     | 1:CA:974:A:H5''    | 1.45                     | 0.99              |
| 13:AN:60:ARG:HD3   | 13:AN:60:ARG:H     | 1.28                     | 0.98              |
| 25:BC:139:THR:HG22 | 25:BC:193:GLU:HB3  | 1.44                     | 0.98              |
| 43:DW:13:ARG:H     | 43:DW:13:ARG:HE    | 1.08                     | 0.98              |
| 23:DB:2377:A:H61   | 36:DO:13:ARG:HH21  | 1.07                     | 0.98              |
| 9:AJ:35:GLN:HB3    | 9:AJ:77:VAL:HG23   | 1.40                     | 0.98              |
| 27:DE:169:VAL:HG13 | 27:DE:170:ARG:H    | 1.29                     | 0.98              |
| 31:DJ:41:LYS:HZ1   | 38:DQ:63:ARG:HD2   | 1.29                     | 0.98              |
| 41:DT:66:LYS:H     | 41:DT:76:ARG:HH21  | 1.11                     | 0.98              |
| 23:DB:858:G:N3     | 23:DB:2268:A:H2'   | 1.78                     | 0.98              |
| 39:BR:78:ARG:HB3   | 39:BR:87:GLN:HA    | 1.45                     | 0.97              |
| 25:DC:48:ILE:HG22  | 25:DC:49:THR:H     | 1.26                     | 0.97              |
| 23:BB:2266:A:H4'   | 23:BB:2267:A:N7    | 1.80                     | 0.97              |
| 50:D3:49:VAL:HG22  | 50:D3:50:SER:H     | 1.28                     | 0.97              |
| 51:D4:11:CYS:HB2   | 51:D4:14:CYS:HB2   | 1.46                     | 0.97              |
| 33:BL:29:LYS:HD2   | 33:BL:31:GLY:H     | 1.27                     | 0.97              |
| 40:BS:6:LYS:HA     | 40:BS:104:THR:HA   | 1.46                     | 0.97              |
| 23:BB:396:G:H4'    | 46:BZ:28:VAL:HG21  | 1.46                     | 0.97              |
| 23:BB:2478:A:H5'   | 51:B4:32:LYS:HD2   | 1.47                     | 0.97              |
| 45:BY:10:ARG:HE    | 45:BY:31:ILE:HG13  | 1.27                     | 0.97              |
| 25:BC:53:ILE:HD13  | 25:BC:218:THR:HG23 | 1.45                     | 0.97              |
| 46:BZ:3:LYS:HB2    | 46:BZ:51:VAL:HG21  | 1.45                     | 0.97              |
| 46:BZ:33:ASN:HB2   | 46:BZ:44:PHE:HB2   | 1.44                     | 0.97              |
| 23:DB:1099:G:C8    | 52:DI:3:LYS:N      | 2.32                     | 0.97              |
| 39:DR:63:VAL:HG22  | 39:DR:64:VAL:H     | 1.28                     | 0.97              |
| 23:BB:482:A:H5''   | 42:BU:43:LYS:HE3   | 1.47                     | 0.97              |
| 32:BK:26:GLY:HA3   | 32:BK:30:ARG:HE    | 1.29                     | 0.97              |
| 40:DS:46:LEU:HA    | 40:DS:49:LYS:HB2   | 1.45                     | 0.97              |
| 41:DT:48:GLN:HA    | 41:DT:53:VAL:HG22  | 1.46                     | 0.97              |
| 23:BB:528:A:N1     | 23:BB:2042:A:H2'   | 1.80                     | 0.97              |
| 23:BB:1450:G:H21   | 23:BB:1452:G:H1    | 1.12                     | 0.97              |
| 22:BA:75:G:H1'     | 24:BV:29:ILE:HD13  | 1.44                     | 0.96              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:BD:170:VAL:HG13 | 26:BD:171:THR:H    | 1.29                     | 0.96              |
| 32:BK:71:ARG:CB    | 32:BK:72:PRO:HD2   | 1.95                     | 0.96              |
| 8:AI:29:ILE:HG22   | 8:AI:64:ILE:HB     | 1.47                     | 0.96              |
| 23:BB:858:G:H21    | 23:BB:2268:A:H3'   | 1.31                     | 0.96              |
| 31:DJ:35:ARG:HH12  | 31:DJ:40:HIS:H     | 0.98                     | 0.96              |
| 45:DY:18:LYS:H     | 45:DY:18:LYS:HD2   | 1.28                     | 0.96              |
| 38:DQ:53:LYS:HE2   | 38:DQ:53:LYS:H     | 1.30                     | 0.96              |
| 28:BF:36:ASN:HB2   | 28:BF:87:LYS:HA    | 1.47                     | 0.96              |
| 31:BJ:81:ILE:HG13  | 31:BJ:82:GLY:H     | 1.26                     | 0.96              |
| 35:BN:113:ILE:HG22 | 35:BN:114:GLU:H    | 1.30                     | 0.96              |
| 1:CA:1320:C:H5''   | 18:CS:2:ARG:HD3    | 1.47                     | 0.96              |
| 31:DJ:124:VAL:HG23 | 31:DJ:125:TYR:H    | 1.27                     | 0.96              |
| 21:CU:17:ARG:HD2   | 21:CU:17:ARG:H     | 1.29                     | 0.96              |
| 51:D4:3:VAL:HG12   | 51:D4:4:ARG:H      | 1.30                     | 0.96              |
| 25:BC:28:PRO:HD2   | 25:BC:79:ARG:HH21  | 1.27                     | 0.96              |
| 1:CA:1003:G:H21    | 1:CA:1005:A:H5'    | 1.27                     | 0.96              |
| 39:BR:74:ILE:HA    | 39:BR:90:ARG:HE    | 1.27                     | 0.96              |
| 23:BB:858:G:N3     | 23:BB:2268:A:H2'   | 1.81                     | 0.96              |
| 10:CK:78:ILE:H     | 10:CK:78:ILE:HD13  | 1.28                     | 0.96              |
| 34:DM:5:LYS:HE3    | 34:DM:6:ARG:N      | 1.80                     | 0.96              |
| 37:DP:25:VAL:HG11  | 37:DP:87:ARG:HA    | 1.47                     | 0.96              |
| 42:DU:66:VAL:HG22  | 42:DU:67:SER:H     | 1.29                     | 0.96              |
| 13:AN:63:CYS:HB3   | 13:AN:67:GLY:H     | 1.30                     | 0.95              |
| 38:BQ:92:LYS:HG2   | 38:BQ:93:ILE:H     | 1.29                     | 0.95              |
| 5:CF:29:ILE:HD13   | 5:CF:64:VAL:HG11   | 1.48                     | 0.95              |
| 46:DZ:54:GLY:H     | 46:DZ:57:VAL:HG23  | 1.31                     | 0.95              |
| 31:DJ:40:HIS:HB2   | 38:DQ:69:ARG:HH22  | 1.29                     | 0.95              |
| 20:CB:156:LEU:HD11 | 20:CB:178:LEU:HD13 | 1.47                     | 0.95              |
| 25:BC:28:PRO:HD2   | 25:BC:79:ARG:NH2   | 1.82                     | 0.95              |
| 23:DB:1368:G:H5''  | 49:D2:25:LYS:HG2   | 1.46                     | 0.95              |
| 7:AH:30:LYS:HZ2    | 7:AH:30:LYS:HA     | 1.32                     | 0.95              |
| 23:BB:1392:A:H62   | 41:BT:18:GLU:HG2   | 1.30                     | 0.95              |
| 41:BT:88:LYS:HG2   | 41:BT:89:GLU:H     | 1.30                     | 0.95              |
| 19:AT:68:LYS:HG3   | 19:AT:69:ASN:H     | 1.29                     | 0.95              |
| 23:BB:2576:G:P     | 26:BD:149:ASN:HB2  | 2.07                     | 0.95              |
| 31:DJ:84:ILE:HD12  | 31:DJ:85:LYS:H     | 1.31                     | 0.95              |
| 27:DE:127:GLU:HA   | 27:DE:157:LEU:HD13 | 1.49                     | 0.95              |
| 5:AF:53:LYS:HD3    | 5:AF:54:LEU:H      | 1.30                     | 0.94              |
| 18:AS:49:ALA:HB1   | 18:AS:56:HIS:HB3   | 1.49                     | 0.94              |
| 12:AM:48:SER:H     | 12:AM:51:GLN:HB2   | 1.33                     | 0.94              |
| 1:CA:437:U:H2'     | 1:CA:438:U:O4'     | 1.67                     | 0.94              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:BS:71:VAL:HG22 | 40:BS:107:VAL:HG12 | 1.45                     | 0.94              |
| 44:BX:24:GLU:HA   | 44:BX:28:LEU:HB2   | 1.47                     | 0.94              |
| 23:DB:2377:A:H61  | 36:DO:13:ARG:NH2   | 1.64                     | 0.94              |
| 46:DZ:30:HIS:HB2  | 46:DZ:48:GLN:HG2   | 1.48                     | 0.94              |
| 1:AA:764:C:H3'    | 1:AA:765:G:H21     | 1.33                     | 0.94              |
| 27:BE:116:ASP:HB2 | 27:BE:185:LYS:HA   | 1.50                     | 0.94              |
| 43:BW:35:ILE:HG23 | 43:BW:36:ILE:H     | 1.32                     | 0.94              |
| 8:CI:118:ARG:HH21 | 8:CI:122:ARG:HE    | 1.13                     | 0.94              |
| 39:DR:65:ALA:HB3  | 39:DR:99:THR:HG23  | 1.48                     | 0.94              |
| 21:AU:3:ILE:HA    | 21:AU:19:LYS:HG2   | 1.50                     | 0.94              |
| 27:BE:47:LYS:HD3  | 27:BE:47:LYS:H     | 1.30                     | 0.94              |
| 34:BM:82:MET:HB2  | 34:BM:84:LYS:HZ2   | 1.30                     | 0.94              |
| 38:BQ:93:ILE:HG23 | 38:BQ:94:LEU:HD13  | 1.50                     | 0.94              |
| 46:BZ:36:VAL:HA   | 46:BZ:42:PRO:HB3   | 1.45                     | 0.94              |
| 51:B4:12:ARG:H    | 51:B4:12:ARG:HD2   | 1.32                     | 0.94              |
| 3:CD:167:PRO:HG2  | 3:CD:170:LEU:HD11  | 1.48                     | 0.94              |
| 23:DB:918:A:H2'   | 23:DB:919:U:H5'    | 1.46                     | 0.94              |
| 10:CK:19:VAL:HG22 | 10:CK:34:THR:HG22  | 1.49                     | 0.94              |
| 34:DM:57:VAL:HG12 | 34:DM:58:LYS:H     | 1.30                     | 0.94              |
| 1:AA:437:U:H2'    | 1:AA:438:U:O4'     | 1.67                     | 0.94              |
| 28:BF:133:GLU:HG2 | 28:BF:147:ARG:HG2  | 1.49                     | 0.94              |
| 37:DP:47:ILE:HG23 | 37:DP:63:ILE:HA    | 1.46                     | 0.94              |
| 24:BV:4:ILE:HB    | 24:BV:63:ILE:HA    | 1.49                     | 0.93              |
| 23:DB:972:A:H3'   | 23:DB:973:A:H5''   | 1.48                     | 0.93              |
| 23:DB:1199:U:H2'  | 23:DB:1200:C:H6    | 1.31                     | 0.93              |
| 1:AA:1313:U:H5''  | 18:AS:5:LYS:HG2    | 1.49                     | 0.93              |
| 13:CN:50:LEU:H    | 13:CN:51:PRO:HD2   | 1.33                     | 0.93              |
| 23:DB:1450:G:H21  | 23:DB:1452:G:H1    | 1.12                     | 0.93              |
| 26:DD:77:ARG:HH21 | 26:DD:79:LEU:HB2   | 1.30                     | 0.93              |
| 30:DH:125:THR:HA  | 30:DH:146:VAL:HB   | 1.51                     | 0.93              |
| 41:BT:54:GLU:H    | 41:BT:91:GLN:HE22  | 1.15                     | 0.93              |
| 23:DB:142:A:H2'   | 23:DB:143:C:C6     | 2.03                     | 0.93              |
| 28:DF:28:PRO:HB2  | 28:DF:168:LEU:HD12 | 1.48                     | 0.93              |
| 44:BX:28:LEU:HB3  | 44:BX:34:SER:HA    | 1.49                     | 0.93              |
| 1:CA:264:C:H4'    | 16:CQ:64:ARG:HD2   | 1.49                     | 0.93              |
| 37:DP:26:GLU:HA   | 37:DP:47:ILE:H     | 1.33                     | 0.93              |
| 12:AM:78:ARG:HH21 | 12:AM:79:LEU:HG    | 1.33                     | 0.93              |
| 23:DB:2304:G:H4'  | 28:DF:129:MET:HA   | 1.48                     | 0.93              |
| 23:DB:2574:G:H21  | 26:DD:147:GLY:HA3  | 1.31                     | 0.93              |
| 38:BQ:33:VAL:HG13 | 38:BQ:34:ALA:H     | 1.31                     | 0.93              |
| 28:DF:32:LYS:HB3  | 28:DF:91:ARG:HB3   | 1.48                     | 0.93              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 10:AK:22:ILE:HG21  | 10:AK:95:THR:HG21 | 1.51                     | 0.93              |
| 14:AO:6:ALA:HA     | 14:AO:9:LYS:HE3   | 1.50                     | 0.93              |
| 33:DL:85:VAL:HG13  | 33:DL:86:GLU:H    | 1.33                     | 0.93              |
| 37:DP:100:ARG:HH11 | 37:DP:100:ARG:HB3 | 1.32                     | 0.93              |
| 23:BB:37:C:H2'     | 27:BE:46:GLN:CG   | 1.99                     | 0.93              |
| 26:BD:16:THR:HG23  | 26:BD:17:GLU:H    | 1.33                     | 0.93              |
| 33:BL:14:LYS:HA    | 33:BL:14:LYS:NZ   | 1.82                     | 0.93              |
| 33:BL:94:THR:HG23  | 33:BL:95:LEU:HD12 | 1.50                     | 0.93              |
| 23:BB:919:U:H2'    | 23:BB:920:A:C8    | 2.05                     | 0.92              |
| 41:BT:8:LEU:HB3    | 44:BX:19:LEU:HD11 | 1.48                     | 0.92              |
| 49:B2:42:LEU:HD11  | 49:B2:44:VAL:HG13 | 1.48                     | 0.92              |
| 2:CC:127:VAL:HB    | 2:CC:128:MET:HE3  | 1.50                     | 0.92              |
| 43:DW:35:ILE:H     | 43:DW:35:ILE:HD12 | 1.34                     | 0.92              |
| 23:BB:480:A:H4'    | 42:BU:42:LYS:HG2  | 1.51                     | 0.92              |
| 32:BK:66:LYS:HG2   | 32:BK:80:ASP:HA   | 1.49                     | 0.92              |
| 46:BZ:25:ARG:HH11  | 46:BZ:25:ARG:HB2  | 1.33                     | 0.92              |
| 23:DB:1099:G:P     | 52:DI:3:LYS:HA    | 2.09                     | 0.92              |
| 23:DB:2046:G:H5'   | 47:D0:15:ARG:HD2  | 1.51                     | 0.92              |
| 23:BB:535:G:H21    | 38:BQ:52:ARG:HH22 | 1.13                     | 0.92              |
| 27:BE:48:THR:HG22  | 27:BE:49:ARG:H    | 1.34                     | 0.92              |
| 33:BL:60:ARG:HA    | 33:BL:60:ARG:HH11 | 1.31                     | 0.92              |
| 22:DA:48:U:H2'     | 22:DA:49:C:C6     | 2.03                     | 0.92              |
| 48:D1:47:ILE:HG22  | 48:D1:48:TYR:H    | 1.34                     | 0.92              |
| 33:BL:90:VAL:HG11  | 33:BL:121:THR:H   | 1.34                     | 0.92              |
| 21:CU:24:LYS:HD2   | 21:CU:25:ALA:H    | 1.34                     | 0.92              |
| 23:DB:1024:G:H3'   | 23:DB:1025:G:H5'' | 1.50                     | 0.92              |
| 28:DF:13:LYS:HA    | 28:DF:16:MET:HB2  | 1.51                     | 0.92              |
| 32:BK:70:ARG:HB3   | 32:BK:76:VAL:HG22 | 1.50                     | 0.92              |
| 39:BR:47:VAL:HG13  | 39:BR:49:ILE:H    | 1.34                     | 0.92              |
| 12:CM:52:ILE:HG13  | 12:CM:56:ARG:HH22 | 1.33                     | 0.92              |
| 23:DB:1099:G:H8    | 52:DI:3:LYS:CA    | 1.83                     | 0.92              |
| 41:DT:76:ARG:HH12  | 41:DT:78:SER:HB2  | 1.35                     | 0.92              |
| 8:AI:51:LEU:HD23   | 8:AI:56:MET:HE3   | 1.49                     | 0.92              |
| 27:BE:143:LEU:HG   | 27:BE:185:LYS:HD2 | 1.51                     | 0.92              |
| 30:BH:134:VAL:HG13 | 30:BH:135:HIS:H   | 1.35                     | 0.92              |
| 26:BD:118:PHE:HA   | 26:BD:164:GLN:HA  | 1.52                     | 0.92              |
| 27:DE:142:ALA:H    | 27:DE:185:LYS:HZ1 | 1.12                     | 0.92              |
| 27:DE:148:ILE:HA   | 27:DE:185:LYS:HB3 | 1.50                     | 0.92              |
| 37:DP:27:VAL:HG13  | 37:DP:47:ILE:HD12 | 1.49                     | 0.92              |
| 1:AA:1086:U:H3     | 1:AA:1099:G:H22   | 1.05                     | 0.92              |
| 23:BB:543:G:H2'    | 23:BB:544:C:H5''  | 1.51                     | 0.92              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:BF:168:LEU:HD12 | 28:BF:169:LEU:H    | 1.35                     | 0.92              |
| 3:CD:58:GLN:HE21   | 3:CD:58:GLN:HA     | 1.35                     | 0.92              |
| 9:CJ:51:VAL:HG23   | 13:CN:80:ARG:HB2   | 1.51                     | 0.92              |
| 26:BD:126:ASN:O    | 26:BD:127:PHE:HB2  | 1.70                     | 0.92              |
| 33:BL:77:ILE:HB    | 33:BL:110:VAL:HG22 | 1.51                     | 0.92              |
| 1:CA:1367:C:H5''   | 8:CI:115:VAL:HG23  | 1.49                     | 0.92              |
| 31:BJ:64:VAL:HG11  | 31:BJ:68:LYS:HD2   | 1.50                     | 0.91              |
| 1:AA:376:G:H5''    | 15:AP:5:ARG:HB2    | 1.52                     | 0.91              |
| 10:AK:124:LYS:HA   | 21:AU:34:ARG:HB3   | 1.49                     | 0.91              |
| 23:BB:630:G:H1     | 33:BL:69:ARG:HH22  | 1.04                     | 0.91              |
| 34:BM:96:ILE:HG23  | 34:BM:97:GLN:H     | 1.35                     | 0.91              |
| 21:CU:4:LYS:HB3    | 21:CU:6:ARG:HH12   | 1.32                     | 0.91              |
| 23:DB:856:G:H4'    | 43:DW:23:LYS:HD2   | 1.52                     | 0.91              |
| 23:DB:2054:A:H2'   | 47:D0:4:GLN:HE22   | 1.35                     | 0.91              |
| 30:DH:26:ALA:HB2   | 30:DH:30:LEU:HG    | 1.49                     | 0.91              |
| 40:DS:23:LEU:HB2   | 47:D0:21:LEU:HD13  | 1.52                     | 0.91              |
| 20:AB:9:LEU:HD22   | 20:AB:11:ALA:H     | 1.33                     | 0.91              |
| 23:BB:1639:C:H2'   | 23:BB:1640:A:H5''  | 1.52                     | 0.91              |
| 33:BL:55:MET:HG2   | 33:BL:56:PRO:HD3   | 1.52                     | 0.91              |
| 23:DB:27:G:H22     | 23:DB:512:G:H2'    | 1.35                     | 0.91              |
| 25:DC:127:ASN:HD22 | 25:DC:128:THR:H    | 1.15                     | 0.91              |
| 31:BJ:45:THR:HB    | 38:BQ:63:ARG:HH22  | 1.35                     | 0.91              |
| 36:DO:40:ILE:HD13  | 36:DO:40:ILE:H     | 1.35                     | 0.91              |
| 41:DT:55:VAL:HG22  | 41:DT:56:GLU:H     | 1.33                     | 0.91              |
| 10:AK:86:LYS:HG3   | 10:AK:113:THR:HA   | 1.53                     | 0.91              |
| 23:BB:1453:A:N6    | 35:BN:74:GLU:HG2   | 1.85                     | 0.91              |
| 38:BQ:91:ARG:H     | 39:BR:10:LYS:HZ2   | 0.93                     | 0.91              |
| 23:DB:360:U:H2'    | 23:DB:361:G:O4'    | 1.70                     | 0.91              |
| 23:BB:670:A:H3'    | 33:BL:47:ARG:HH11  | 1.32                     | 0.91              |
| 27:DE:4:VAL:HG13   | 27:DE:5:LEU:H      | 1.36                     | 0.91              |
| 10:CK:20:ALA:HB3   | 10:CK:83:VAL:HA    | 1.53                     | 0.91              |
| 23:DB:1099:G:O4'   | 52:DI:3:LYS:C      | 2.14                     | 0.91              |
| 30:BH:5:LEU:HD22   | 30:BH:5:LEU:H      | 1.35                     | 0.91              |
| 1:CA:764:C:H3'     | 1:CA:765:G:H21     | 1.33                     | 0.91              |
| 2:CC:59:PRO:HG2    | 2:CC:62:SER:HB2    | 1.49                     | 0.91              |
| 31:DJ:81:ILE:HG23  | 31:DJ:82:GLY:H     | 1.34                     | 0.91              |
| 40:DS:29:VAL:HG22  | 40:DS:71:VAL:HG23  | 1.50                     | 0.91              |
| 50:D3:12:ARG:HB3   | 50:D3:23:HIS:HB2   | 1.52                     | 0.91              |
| 50:B3:12:ARG:HB3   | 50:B3:23:HIS:HA    | 1.53                     | 0.91              |
| 36:DO:66:GLY:H     | 36:DO:70:ALA:HB2   | 1.34                     | 0.91              |
| 6:AG:125:ASP:HB3   | 6:AG:130:LYS:HB3   | 1.53                     | 0.90              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:DP:47:ILE:HG12  | 37:DP:63:ILE:HG23  | 1.52                     | 0.90              |
| 26:DD:29:VAL:HG22  | 26:DD:30:GLU:H     | 1.36                     | 0.90              |
| 26:BD:115:GLY:HA2  | 26:BD:165:MET:HG3  | 1.53                     | 0.90              |
| 51:D4:18:LYS:HE2   | 51:D4:19:ARG:N     | 1.86                     | 0.90              |
| 21:AU:13:VAL:HG13  | 21:AU:14:ALA:H     | 1.35                     | 0.90              |
| 27:BE:60:TRP:HE1   | 27:BE:73:ILE:HD11  | 1.34                     | 0.90              |
| 49:B2:44:VAL:HG23  | 49:B2:45:SER:H     | 1.37                     | 0.90              |
| 23:DB:1060:U:N3    | 23:DB:1088:A:N7    | 2.20                     | 0.90              |
| 32:DK:78:ARG:HH22  | 37:DP:62:LYS:HZ2   | 1.16                     | 0.90              |
| 23:BB:691:C:O2'    | 25:BC:42:ARG:HD2   | 1.70                     | 0.90              |
| 23:BB:811:U:H2'    | 33:BL:31:GLY:HA3   | 1.53                     | 0.90              |
| 25:BC:30:ALA:H     | 25:BC:31:PRO:HD3   | 1.36                     | 0.90              |
| 38:BQ:5:ARG:HB2    | 38:BQ:5:ARG:HH11   | 1.34                     | 0.90              |
| 25:DC:224:MET:HA   | 25:DC:233:GLY:H    | 1.36                     | 0.90              |
| 2:AC:156:LEU:HD12  | 2:AC:156:LEU:H     | 1.33                     | 0.90              |
| 25:BC:143:VAL:HG12 | 25:BC:144:GLU:H    | 1.35                     | 0.90              |
| 1:CA:451:A:H5'     | 15:CP:70:ARG:HH22  | 1.35                     | 0.90              |
| 1:CA:719:C:H1'     | 17:CR:37:LYS:HB2   | 1.52                     | 0.90              |
| 23:DB:2645:G:H3'   | 23:DB:2646:C:H5'   | 1.54                     | 0.90              |
| 28:DF:140:ILE:H    | 28:DF:140:ILE:HD12 | 1.37                     | 0.90              |
| 50:D3:51:LYS:HZ2   | 50:D3:51:LYS:HA    | 1.37                     | 0.90              |
| 37:BP:50:ARG:HB2   | 37:BP:50:ARG:HH11  | 1.33                     | 0.90              |
| 18:CS:29:PRO:HA    | 18:CS:47:THR:HB    | 1.54                     | 0.90              |
| 50:B3:24:LYS:HA    | 50:B3:45:PRO:HB3   | 1.54                     | 0.90              |
| 20:CB:15:PHE:HA    | 20:CB:42:LEU:HD21  | 1.51                     | 0.90              |
| 27:DE:149:ILE:HD13 | 27:DE:186:VAL:HG13 | 1.54                     | 0.90              |
| 50:D3:32:LEU:HD13  | 50:D3:33:THR:H     | 1.35                     | 0.90              |
| 32:BK:103:VAL:HB   | 32:BK:107:LEU:HD23 | 1.54                     | 0.90              |
| 41:DT:31:VAL:HG13  | 41:DT:32:LEU:H     | 1.37                     | 0.90              |
| 1:AA:1211:U:H4'    | 1:AA:1213:A:H1'    | 1.54                     | 0.89              |
| 20:AB:202:ASN:HD22 | 20:AB:204:ASP:H    | 1.20                     | 0.89              |
| 23:BB:1283:G:H22   | 23:BB:1286:A:H5'   | 1.36                     | 0.89              |
| 34:BM:3:GLN:N      | 34:BM:4:PRO:HD2    | 1.82                     | 0.89              |
| 40:BS:27:LYS:HD2   | 40:BS:27:LYS:H     | 1.33                     | 0.89              |
| 5:CF:38:ARG:HH11   | 5:CF:98:GLU:H      | 1.18                     | 0.89              |
| 31:DJ:98:GLU:HB3   | 31:DJ:124:VAL:HB   | 1.51                     | 0.89              |
| 7:AH:103:VAL:HG12  | 7:AH:124:ILE:HA    | 1.53                     | 0.89              |
| 23:BB:2575:C:H4'   | 26:BD:148:GLN:HA   | 1.54                     | 0.89              |
| 31:BJ:78:THR:H     | 31:BJ:84:ILE:HG21  | 1.35                     | 0.89              |
| 34:BM:70:ASP:N     | 34:BM:71:LYS:HZ2   | 1.69                     | 0.89              |
| 45:BY:9:THR:HA     | 45:BY:55:LYS:HE2   | 1.53                     | 0.89              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:DJ:58:ASN:O     | 31:DJ:126:ALA:HA   | 1.71                     | 0.89              |
| 44:DX:18:LEU:HD22  | 44:DX:18:LEU:H     | 1.36                     | 0.89              |
| 23:BB:855:G:N2     | 43:BW:23:LYS:HD2   | 1.86                     | 0.89              |
| 23:BB:2645:G:H3'   | 23:BB:2646:C:H5'   | 1.54                     | 0.89              |
| 23:BB:45:G:H5'     | 23:BB:46:G:H5'     | 1.53                     | 0.89              |
| 26:BD:2:ILE:HG21   | 26:BD:204:LYS:HA   | 1.52                     | 0.89              |
| 41:BT:58:VAL:HG13  | 41:BT:85:VAL:HG12  | 1.51                     | 0.89              |
| 52:BI:27:LEU:HD23  | 52:BI:27:LEU:H     | 1.37                     | 0.89              |
| 23:DB:161:A:H3'    | 23:DB:162:U:H5''   | 1.53                     | 0.89              |
| 24:DV:25:LYS:HE2   | 24:DV:41:GLU:HB2   | 1.54                     | 0.89              |
| 5:CF:6:ILE:HG23    | 5:CF:62:MET:HB3    | 1.52                     | 0.89              |
| 34:DM:18:ARG:HD3   | 34:DM:18:ARG:H     | 1.36                     | 0.89              |
| 46:BZ:5:ILE:HD12   | 46:BZ:5:ILE:H      | 1.37                     | 0.89              |
| 25:DC:50:THR:HG22  | 25:DC:51:ARG:HG3   | 1.52                     | 0.89              |
| 25:BC:229:HIS:NE2  | 25:BC:244:VAL:HG22 | 1.88                     | 0.89              |
| 33:BL:77:ILE:HD13  | 33:BL:92:LEU:HD13  | 1.52                     | 0.89              |
| 23:DB:1283:G:H22   | 23:DB:1286:A:H5'   | 1.36                     | 0.89              |
| 30:DH:86:ASP:HB2   | 30:DH:89:LYS:HD3   | 1.55                     | 0.89              |
| 23:BB:1060:U:N3    | 23:BB:1088:A:N7    | 2.20                     | 0.89              |
| 33:BL:30:THR:HB    | 33:BL:36:LYS:HB2   | 1.55                     | 0.89              |
| 34:BM:33:LEU:HD22  | 34:BM:124:LEU:HG   | 1.54                     | 0.89              |
| 1:CA:699:C:C2'     | 1:CA:700:G:H5''    | 2.02                     | 0.89              |
| 23:DB:2156:G:H2'   | 23:DB:2157:G:H4'   | 1.53                     | 0.89              |
| 23:DB:2839:G:H4'   | 35:DN:49:GLU:HG2   | 1.55                     | 0.89              |
| 50:B3:15:LYS:HG2   | 50:B3:19:GLY:HA2   | 1.55                     | 0.89              |
| 5:CF:3:HIS:HA      | 5:CF:65:GLU:HG3    | 1.54                     | 0.89              |
| 13:CN:26:LEU:HG    | 13:CN:44:VAL:HG22  | 1.55                     | 0.89              |
| 23:DB:919:U:H2'    | 23:DB:920:A:C8     | 2.07                     | 0.89              |
| 23:DB:1639:C:H2'   | 23:DB:1640:A:H5''  | 1.52                     | 0.89              |
| 23:BB:654:A:H2'    | 23:BB:655:A:H5''   | 1.55                     | 0.88              |
| 37:DP:27:VAL:HA    | 37:DP:86:LYS:HE2   | 1.53                     | 0.88              |
| 23:BB:535:G:H21    | 38:BQ:52:ARG:NH2   | 1.70                     | 0.88              |
| 23:BB:2641:G:H5''  | 31:BJ:78:THR:HG21  | 1.53                     | 0.88              |
| 32:BK:99:ILE:HG12  | 32:BK:115:ILE:HG13 | 1.52                     | 0.88              |
| 33:BL:118:THR:HG23 | 33:BL:119:PRO:HD3  | 1.53                     | 0.88              |
| 43:BW:48:ALA:HA    | 43:BW:54:ARG:H     | 1.38                     | 0.88              |
| 11:CL:23:LEU:HD22  | 11:CL:58:ASN:HD22  | 1.38                     | 0.88              |
| 1:AA:699:C:C2'     | 1:AA:700:G:H5''    | 2.02                     | 0.88              |
| 30:BH:21:VAL:HG22  | 30:BH:22:LYS:H     | 1.38                     | 0.88              |
| 42:BU:12:VAL:HA    | 42:BU:68:ASN:HD21  | 1.38                     | 0.88              |
| 23:DB:2751:G:H5'   | 29:DG:3:VAL:HG21   | 1.53                     | 0.88              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:DM:41:LEU:HD22 | 34:DM:95:LEU:HD13  | 1.53                     | 0.88              |
| 11:AL:48:LEU:HD23 | 11:AL:48:LEU:H     | 1.34                     | 0.88              |
| 23:BB:1021:A:H62  | 23:BB:1141:U:H3    | 1.18                     | 0.88              |
| 26:BD:70:LYS:HA   | 26:BD:70:LYS:HE3   | 1.54                     | 0.88              |
| 33:DL:51:GLU:HG2  | 33:DL:52:GLY:N     | 1.88                     | 0.88              |
| 50:B3:12:ARG:NH1  | 50:B3:12:ARG:HB2   | 1.87                     | 0.88              |
| 1:AA:74:A:C2'     | 1:AA:75:G:H5''     | 2.04                     | 0.88              |
| 25:BC:67:LYS:HG3  | 25:BC:68:ARG:H     | 1.37                     | 0.88              |
| 28:DF:128:SER:HB3 | 28:DF:154:THR:HG23 | 1.56                     | 0.88              |
| 35:DN:5:LYS:HE2   | 35:DN:5:LYS:HA     | 1.55                     | 0.88              |
| 23:BB:1141:U:H4'  | 23:BB:1142:A:O4'   | 1.74                     | 0.88              |
| 26:BD:34:VAL:HA   | 26:BD:89:GLU:HB2   | 1.53                     | 0.88              |
| 33:BL:64:PHE:H    | 50:B3:24:LYS:HD2   | 1.36                     | 0.88              |
| 34:DM:29:GLY:H    | 34:DM:102:LEU:HD12 | 1.38                     | 0.88              |
| 33:DL:126:ARG:O   | 33:DL:127:VAL:HG22 | 1.74                     | 0.88              |
| 44:DX:43:LEU:HB2  | 44:DX:45:GLN:NE2   | 1.89                     | 0.88              |
| 33:BL:79:LEU:HB3  | 33:BL:114:GLY:H    | 1.35                     | 0.88              |
| 35:BN:76:VAL:HA   | 35:BN:79:LEU:HD12  | 1.56                     | 0.88              |
| 23:DB:929:U:H4'   | 45:DY:2:LYS:HE3    | 1.54                     | 0.88              |
| 37:DP:32:VAL:HA   | 37:DP:42:PHE:HB3   | 1.55                     | 0.88              |
| 23:BB:396:G:H5'   | 46:BZ:9:TYR:HB2    | 1.54                     | 0.88              |
| 26:BD:5:VAL:HG11  | 26:BD:28:GLU:HA    | 1.54                     | 0.88              |
| 30:BH:4:ILE:H     | 30:BH:37:VAL:HB    | 1.39                     | 0.88              |
| 34:BM:38:ARG:HB2  | 34:BM:38:ARG:NH1   | 1.89                     | 0.88              |
| 39:BR:37:GLU:HG2  | 39:BR:62:GLU:H     | 1.38                     | 0.88              |
| 45:BY:15:ARG:HB3  | 45:BY:18:LYS:HE3   | 1.56                     | 0.88              |
| 13:CN:30:ILE:HG21 | 13:CN:43:ALA:HB3   | 1.55                     | 0.88              |
| 23:DB:1141:U:H4'  | 23:DB:1142:A:O4'   | 1.74                     | 0.88              |
| 1:AA:1409:C:N4    | 1:AA:1491:G:H1     | 1.72                     | 0.87              |
| 32:DK:108:ARG:HA  | 32:DK:116:ILE:HD13 | 1.56                     | 0.87              |
| 35:DN:24:MET:HE1  | 35:DN:36:THR:HG21  | 1.54                     | 0.87              |
| 37:BP:47:ILE:HG22 | 37:BP:48:ALA:H     | 1.37                     | 0.87              |
| 43:BW:28:GLU:H    | 43:BW:61:LYS:HB2   | 1.37                     | 0.87              |
| 23:DB:654:A:H2'   | 23:DB:655:A:H5''   | 1.54                     | 0.87              |
| 39:DR:39:LEU:H    | 39:DR:61:ALA:HB1   | 1.39                     | 0.87              |
| 39:DR:89:HIS:O    | 39:DR:90:ARG:HG3   | 1.74                     | 0.87              |
| 38:BQ:91:ARG:H    | 39:BR:10:LYS:NZ    | 1.73                     | 0.87              |
| 41:BT:5:GLU:HG2   | 41:BT:6:ARG:H      | 1.40                     | 0.87              |
| 27:DE:49:ARG:HG3  | 27:DE:52:VAL:HG22  | 1.56                     | 0.87              |
| 5:AF:38:ARG:HB3   | 5:AF:63:ASN:HB2    | 1.55                     | 0.87              |
| 23:BB:37:C:H2'    | 27:BE:46:GLN:CD    | 1.99                     | 0.87              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:DL:124:GLY:H    | 33:DL:142:ILE:HA   | 1.37                     | 0.87              |
| 2:AC:146:LYS:HD3   | 2:AC:204:GLY:HA2   | 1.56                     | 0.87              |
| 23:BB:2147:A:H5'   | 23:BB:2148:G:H5'   | 1.55                     | 0.87              |
| 42:BU:84:PHE:HB3   | 42:BU:92:VAL:HG22  | 1.57                     | 0.87              |
| 23:DB:2032:G:N3    | 26:DD:150:GLN:HG2  | 1.90                     | 0.87              |
| 26:DD:69:ALA:HB1   | 26:DD:92:VAL:HG13  | 1.56                     | 0.87              |
| 29:BG:29:ASN:HB2   | 29:BG:78:VAL:HA    | 1.57                     | 0.87              |
| 43:BW:19:ARG:HH22  | 43:BW:71:LYS:HD3   | 1.38                     | 0.87              |
| 1:CA:1306:A:N6     | 1:CA:1331:G:H1'    | 1.89                     | 0.87              |
| 26:DD:96:ILE:HG22  | 26:DD:98:VAL:H     | 1.35                     | 0.87              |
| 27:DE:116:ASP:HB3  | 27:DE:185:LYS:HA   | 1.56                     | 0.87              |
| 4:CE:19:ARG:HG2    | 4:CE:20:VAL:H      | 1.39                     | 0.87              |
| 23:DB:1199:U:H2'   | 23:DB:1200:C:C6    | 2.09                     | 0.87              |
| 40:BS:34:ASP:H     | 40:BS:37:THR:HG22  | 1.40                     | 0.87              |
| 42:BU:40:LEU:HD13  | 42:BU:41:VAL:N     | 1.88                     | 0.87              |
| 1:CA:1250:A:H4'    | 8:CI:69:GLY:H      | 1.38                     | 0.87              |
| 23:BB:2052:A:H4'   | 26:BD:148:GLN:N    | 1.90                     | 0.87              |
| 23:BB:2354:C:H4'   | 43:BW:30:VAL:HG22  | 1.57                     | 0.87              |
| 42:BU:23:LYS:HG3   | 42:BU:24:VAL:HG23  | 1.55                     | 0.87              |
| 23:DB:1813:G:N3    | 25:DC:50:THR:HG21  | 1.89                     | 0.87              |
| 31:DJ:64:VAL:HG12  | 31:DJ:65:THR:H     | 1.37                     | 0.87              |
| 37:DP:76:HIS:CD2   | 37:DP:76:HIS:H     | 1.89                     | 0.87              |
| 43:DW:47:GLY:HA2   | 43:DW:71:LYS:HB3   | 1.57                     | 0.87              |
| 1:AA:1323:G:H2'    | 1:AA:1324:A:C8     | 2.09                     | 0.86              |
| 23:BB:547:A:H3'    | 23:BB:548:G:H8     | 1.40                     | 0.86              |
| 21:CU:34:ARG:HG2   | 21:CU:35:GLU:H     | 1.39                     | 0.86              |
| 7:AH:113:ARG:HH21  | 7:AH:114:ALA:HA    | 1.39                     | 0.86              |
| 21:AU:36:PHE:HB3   | 21:AU:40:PRO:HD3   | 1.57                     | 0.86              |
| 31:BJ:100:VAL:HG13 | 31:BJ:101:ILE:HG22 | 1.53                     | 0.86              |
| 5:AF:64:VAL:HG12   | 5:AF:65:GLU:H      | 1.40                     | 0.86              |
| 26:DD:152:PRO:HB2  | 26:DD:154:LYS:HE2  | 1.58                     | 0.86              |
| 51:D4:26:ILE:HG23  | 51:D4:27:CYS:H     | 1.40                     | 0.86              |
| 42:BU:43:LYS:HA    | 42:BU:57:ILE:HA    | 1.57                     | 0.86              |
| 3:CD:25:ARG:HB2    | 3:CD:25:ARG:HH11   | 1.40                     | 0.86              |
| 10:CK:88:PRO:HD3   | 21:CU:28:LEU:HD13  | 1.56                     | 0.86              |
| 45:DY:2:LYS:HB2    | 45:DY:37:ARG:HB2   | 1.56                     | 0.86              |
| 8:CI:51:LEU:HB3    | 8:CI:56:MET:HG2    | 1.58                     | 0.86              |
| 1:AA:1422:G:H5'    | 32:BK:48:PRO:HB3   | 1.58                     | 0.86              |
| 23:BB:479:A:O2'    | 23:BB:481:G:H5'    | 1.75                     | 0.86              |
| 25:BC:124:LYS:HB2  | 25:BC:125:PRO:CD   | 2.05                     | 0.86              |
| 48:B1:46:VAL:HG13  | 48:B1:47:ILE:HG12  | 1.54                     | 0.86              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:CD:63:ILE:HG23   | 3:CD:64:TYR:HD1    | 1.40                     | 0.86              |
| 18:CS:10:ILE:HG22  | 18:CS:37:SER:HB2   | 1.57                     | 0.86              |
| 6:AG:21:LEU:HD23   | 6:AG:21:LEU:H      | 1.41                     | 0.86              |
| 23:BB:703:U:H2'    | 23:BB:704:G:O4'    | 1.76                     | 0.86              |
| 26:BD:130:GLN:NE2  | 26:BD:138:LEU:HD12 | 1.91                     | 0.86              |
| 11:CL:43:LYS:HB3   | 11:CL:44:PRO:CD    | 2.06                     | 0.86              |
| 36:BO:49:VAL:HG22  | 36:BO:50:ALA:H     | 1.38                     | 0.86              |
| 23:DB:1098:A:H2'   | 52:DI:4:VAL:N      | 1.90                     | 0.86              |
| 38:DQ:97:ILE:HD12  | 39:DR:13:ARG:HD2   | 1.58                     | 0.86              |
| 7:CH:105:THR:HA    | 7:CH:122:GLY:HA3   | 1.57                     | 0.86              |
| 33:DL:115:GLU:O    | 33:DL:116:VAL:HG22 | 1.76                     | 0.86              |
| 42:DU:60:LYS:HE3   | 42:DU:61:GLU:N     | 1.91                     | 0.86              |
| 11:AL:35:ARG:NH2   | 11:AL:75:GLU:HB3   | 1.89                     | 0.86              |
| 15:AP:51:ARG:HB3   | 15:AP:51:ARG:NH1   | 1.91                     | 0.86              |
| 31:BJ:3:THR:HG21   | 38:BQ:93:ILE:HG13  | 1.56                     | 0.86              |
| 46:BZ:8:LYS:HD2    | 46:BZ:9:TYR:N      | 1.91                     | 0.86              |
| 25:BC:19:VAL:HG12  | 25:BC:20:ASN:H     | 1.38                     | 0.85              |
| 39:BR:41:ILE:O     | 39:BR:54:VAL:HG13  | 1.74                     | 0.85              |
| 25:DC:51:ARG:HH12  | 25:DC:54:GLY:HA3   | 1.40                     | 0.85              |
| 23:BB:135:U:H2'    | 23:BB:136:G:C8     | 2.11                     | 0.85              |
| 46:BZ:13:THR:HG23  | 46:BZ:25:ARG:HB3   | 1.56                     | 0.85              |
| 9:CJ:6:ILE:HD11    | 9:CJ:79:PRO:HB3    | 1.58                     | 0.85              |
| 11:CL:98:ARG:HG3   | 11:CL:105:GLY:HA2  | 1.56                     | 0.85              |
| 33:DL:118:THR:O    | 33:DL:120:VAL:HG23 | 1.75                     | 0.85              |
| 25:BC:74:PRO:HB2   | 25:BC:96:LYS:HG3   | 1.57                     | 0.85              |
| 26:BD:22:ILE:N     | 26:BD:23:PRO:HD3   | 1.92                     | 0.85              |
| 35:BN:44:LEU:HD23  | 35:BN:113:ILE:HG13 | 1.56                     | 0.85              |
| 20:CB:116:LEU:HD22 | 20:CB:140:LEU:HD21 | 1.59                     | 0.85              |
| 25:DC:220:ARG:CZ   | 25:DC:220:ARG:HA   | 2.07                     | 0.85              |
| 26:DD:31:ALA:HA    | 26:DD:51:THR:HA    | 1.58                     | 0.85              |
| 43:DW:38:ARG:NH2   | 43:DW:40:ARG:HD3   | 1.91                     | 0.85              |
| 52:DI:27:LEU:H     | 52:DI:27:LEU:HD23  | 1.37                     | 0.85              |
| 23:BB:2052:A:C4'   | 26:BD:148:GLN:H    | 1.88                     | 0.85              |
| 4:CE:89:THR:HG22   | 4:CE:91:SER:H      | 1.41                     | 0.85              |
| 19:CT:68:LYS:HE2   | 19:CT:68:LYS:HA    | 1.57                     | 0.85              |
| 23:DB:1149:G:H2'   | 23:DB:1150:C:C6    | 2.12                     | 0.85              |
| 26:DD:204:LYS:HB3  | 26:DD:205:PRO:HD2  | 1.57                     | 0.85              |
| 32:DK:70:ARG:HD3   | 32:DK:76:VAL:HG22  | 1.59                     | 0.85              |
| 37:DP:38:ARG:HG3   | 37:DP:39:LEU:H     | 1.39                     | 0.85              |
| 33:BL:29:LYS:HD2   | 33:BL:30:THR:H     | 1.42                     | 0.85              |
| 1:CA:1296:C:H4'    | 1:CA:1302:C:N4     | 1.91                     | 0.85              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:CP:28:ARG:HD3   | 15:CP:29:ASN:H     | 1.41                     | 0.85              |
| 20:CB:101:THR:HA   | 20:CB:178:LEU:HD21 | 1.58                     | 0.85              |
| 26:DD:32:ASN:HB3   | 26:DD:91:THR:HA    | 1.58                     | 0.85              |
| 34:DM:62:LYS:H     | 34:DM:104:GLU:HB3  | 1.41                     | 0.85              |
| 1:AA:664:G:H22     | 1:AA:741:G:H1      | 1.23                     | 0.85              |
| 23:DB:2502:G:H5'   | 23:DB:2503:A:H5''  | 1.57                     | 0.85              |
| 37:DP:25:VAL:HG22  | 37:DP:89:GLY:H     | 1.40                     | 0.85              |
| 6:AG:97:ALA:HA     | 6:AG:100:MET:HE3   | 1.58                     | 0.85              |
| 20:AB:163:ILE:HG23 | 20:AB:164:ASP:N    | 1.92                     | 0.85              |
| 1:CA:1008:U:H5''   | 13:CN:23:ARG:HH21  | 1.41                     | 0.85              |
| 9:AJ:35:GLN:HB2    | 9:AJ:78:GLU:HB2    | 1.57                     | 0.85              |
| 34:BM:7:THR:HG22   | 34:BM:8:LYS:H      | 1.41                     | 0.85              |
| 1:CA:1306:A:H61    | 1:CA:1331:G:H1'    | 1.40                     | 0.85              |
| 2:CC:69:THR:HG22   | 2:CC:71:ARG:H      | 1.38                     | 0.85              |
| 19:AT:30:PHE:HB3   | 19:AT:53:MET:HB3   | 1.59                     | 0.85              |
| 28:DF:107:VAL:HG12 | 28:DF:108:PRO:HD3  | 1.57                     | 0.85              |
| 6:AG:112:ASP:HB2   | 6:AG:118:ARG:HG2   | 1.58                     | 0.85              |
| 31:BJ:101:ILE:HG23 | 31:BJ:102:GLU:H    | 1.42                     | 0.85              |
| 14:CO:69:LEU:HD11  | 14:CO:76:ARG:HB3   | 1.57                     | 0.85              |
| 27:DE:3:LEU:HD22   | 27:DE:119:ILE:HD11 | 1.57                     | 0.85              |
| 31:DJ:35:ARG:NH1   | 31:DJ:40:HIS:H     | 1.75                     | 0.85              |
| 33:BL:77:ILE:HG13  | 33:BL:108:ALA:HB1  | 1.59                     | 0.84              |
| 26:DD:14:ILE:HD12  | 37:DP:78:PRO:HG2   | 1.59                     | 0.84              |
| 39:DR:47:VAL:HG22  | 39:DR:48:LYS:H     | 1.40                     | 0.84              |
| 43:DW:67:LYS:HG2   | 43:DW:71:LYS:HB2   | 1.59                     | 0.84              |
| 29:BG:15:ASP:HB3   | 29:BG:26:LYS:HB2   | 1.58                     | 0.84              |
| 1:CA:9:G:H5'       | 4:CE:107:GLY:HA3   | 1.55                     | 0.84              |
| 1:CA:664:G:H22     | 1:CA:741:G:H1      | 1.23                     | 0.84              |
| 3:CD:28:ASP:HB3    | 3:CD:33:ILE:HD12   | 1.58                     | 0.84              |
| 10:AK:126:ARG:HB2  | 21:AU:33:ARG:HD2   | 1.59                     | 0.84              |
| 34:BM:70:ASP:H     | 34:BM:71:LYS:HZ2   | 1.23                     | 0.84              |
| 1:CA:840:C:H2'     | 1:CA:842:U:H5''    | 1.60                     | 0.84              |
| 23:DB:1099:G:H5''  | 52:DI:2:LYS:C      | 2.01                     | 0.84              |
| 1:AA:1101:A:H4'    | 1:AA:1102:A:O5'    | 1.75                     | 0.84              |
| 12:AM:33:LEU:HD22  | 12:AM:38:ILE:HB    | 1.59                     | 0.84              |
| 23:BB:662:G:H4'    | 33:BL:24:GLY:N     | 1.92                     | 0.84              |
| 28:BF:37:MET:HE3   | 28:BF:56:LEU:HD12  | 1.59                     | 0.84              |
| 36:BO:16:ARG:HE    | 36:BO:16:ARG:HA    | 1.42                     | 0.84              |
| 15:CP:67:ILE:HG13  | 15:CP:71:VAL:HG13  | 1.59                     | 0.84              |
| 20:CB:16:GLY:HA3   | 20:CB:39:ILE:HA    | 1.59                     | 0.84              |
| 26:DD:122:VAL:HA   | 26:DD:128:ARG:HG3  | 1.59                     | 0.84              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:74:A:H2'      | 1:AA:75:G:H5''     | 1.58                     | 0.84              |
| 23:BB:2306:C:H42   | 28:BF:38:GLY:H     | 1.24                     | 0.84              |
| 23:BB:2502:G:H5'   | 23:BB:2503:A:H5''  | 1.57                     | 0.84              |
| 26:BD:38:LYS:HG2   | 26:BD:39:ASP:H     | 1.42                     | 0.84              |
| 11:CL:68:GLY:HA3   | 11:CL:106:VAL:HG21 | 1.59                     | 0.84              |
| 15:CP:44:SER:HB3   | 15:CP:46:LYS:HG2   | 1.60                     | 0.84              |
| 21:CU:39:LYS:H     | 21:CU:40:PRO:HD2   | 1.43                     | 0.84              |
| 23:DB:443:A:OP1    | 27:DE:40:ARG:HA    | 1.76                     | 0.84              |
| 1:AA:840:C:H2'     | 1:AA:842:U:H5''    | 1.59                     | 0.84              |
| 6:AG:3:ARG:NH1     | 6:AG:3:ARG:HB3     | 1.92                     | 0.84              |
| 27:BE:128:ALA:CB   | 27:BE:129:PRO:HD3  | 2.07                     | 0.84              |
| 1:CA:781:A:H2'     | 1:CA:782:A:H5'     | 1.60                     | 0.84              |
| 23:DB:1021:A:H61   | 23:DB:1142:A:N6    | 1.73                     | 0.84              |
| 12:AM:15:VAL:HG23  | 12:AM:33:LEU:HD12  | 1.60                     | 0.84              |
| 44:DX:18:LEU:HA    | 44:DX:22:LEU:HD12  | 1.58                     | 0.84              |
| 46:DZ:24:ILE:HD13  | 46:DZ:24:ILE:H     | 1.41                     | 0.84              |
| 14:AO:25:GLU:HG3   | 14:AO:80:LEU:HD12  | 1.59                     | 0.84              |
| 19:AT:27:MET:HE1   | 19:AT:66:ILE:HG12  | 1.59                     | 0.84              |
| 23:BB:2619:C:H5'   | 26:BD:157:LYS:HE2  | 1.59                     | 0.84              |
| 35:BN:101:GLY:HA2  | 35:BN:109:PRO:HA   | 1.58                     | 0.84              |
| 37:BP:59:THR:HG23  | 37:BP:76:HIS:CD2   | 2.12                     | 0.84              |
| 27:DE:47:LYS:HE3   | 27:DE:52:VAL:HG23  | 1.60                     | 0.84              |
| 30:DH:37:VAL:H     | 30:DH:38:PRO:HD2   | 1.43                     | 0.84              |
| 31:DJ:135:GLN:HE22 | 31:DJ:137:PRO:HB2  | 1.43                     | 0.84              |
| 10:AK:86:LYS:HB2   | 10:AK:112:VAL:HG23 | 1.59                     | 0.84              |
| 38:BQ:30:VAL:HG12  | 38:BQ:32:ARG:H     | 1.43                     | 0.84              |
| 38:BQ:92:LYS:CG    | 38:BQ:93:ILE:H     | 1.90                     | 0.84              |
| 11:CL:84:GLY:H     | 11:CL:94:TYR:HA    | 1.42                     | 0.84              |
| 23:DB:2811:G:H5'   | 26:DD:62:LYS:HZ1   | 1.43                     | 0.84              |
| 3:AD:84:ASN:HD22   | 3:AD:87:GLU:H      | 1.26                     | 0.84              |
| 23:BB:2024:G:H4'   | 26:BD:154:LYS:HD3  | 1.60                     | 0.84              |
| 25:BC:155:ARG:HE   | 25:BC:157:ALA:HB3  | 1.41                     | 0.84              |
| 28:BF:66:ILE:HG22  | 28:BF:83:PRO:HB2   | 1.59                     | 0.84              |
| 33:BL:116:VAL:HG12 | 33:BL:117:THR:H    | 1.42                     | 0.84              |
| 42:BU:3:LYS:HB2    | 42:BU:3:LYS:HZ2    | 1.41                     | 0.84              |
| 1:CA:1422:G:H5''   | 32:DK:48:PRO:HB3   | 1.57                     | 0.84              |
| 23:DB:1799:G:N7    | 25:DC:178:GLY:HA3  | 1.92                     | 0.84              |
| 1:AA:33:A:H1'      | 11:AL:27:PRO:HG3   | 1.59                     | 0.83              |
| 1:AA:1330:U:H2'    | 1:AA:1331:G:H5'    | 1.59                     | 0.83              |
| 24:BV:80:HIS:CD2   | 24:BV:83:LYS:H     | 1.94                     | 0.83              |
| 30:BH:130:VAL:HB   | 30:BH:142:VAL:HB   | 1.60                     | 0.83              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:108:G:O6      | 19:CT:9:ARG:HG2    | 1.78                     | 0.83              |
| 2:CC:179:ALA:HA    | 2:CC:205:GLU:HA    | 1.59                     | 0.83              |
| 30:DH:10:ALA:O     | 30:DH:11:ASN:HB3   | 1.78                     | 0.83              |
| 12:AM:3:ILE:HA     | 12:AM:56:ARG:HG2   | 1.60                     | 0.83              |
| 16:AQ:67:SER:HB2   | 16:AQ:70:LYS:HB3   | 1.60                     | 0.83              |
| 35:BN:19:ALA:HA    | 35:BN:22:ARG:HG2   | 1.58                     | 0.83              |
| 8:CI:54:VAL:HG11   | 8:CI:86:LEU:HD13   | 1.58                     | 0.83              |
| 10:CK:113:THR:HG21 | 21:CU:28:LEU:HD11  | 1.59                     | 0.83              |
| 20:AB:33:ALA:HA    | 20:AB:38:HIS:HA    | 1.60                     | 0.83              |
| 25:BC:136:VAL:HG12 | 25:BC:165:ALA:HA   | 1.60                     | 0.83              |
| 20:CB:113:LEU:HD12 | 20:CB:143:LEU:HD22 | 1.60                     | 0.83              |
| 23:DB:2314:A:H1'   | 28:DF:154:THR:HG21 | 1.60                     | 0.83              |
| 28:DF:70:ARG:HA    | 28:DF:80:GLN:HE21  | 1.42                     | 0.83              |
| 30:DH:31:VAL:HB    | 30:DH:32:PRO:HD3   | 1.60                     | 0.83              |
| 37:DP:52:ARG:HB3   | 37:DP:60:VAL:HG11  | 1.60                     | 0.83              |
| 13:AN:30:ILE:H     | 13:AN:30:ILE:HD12  | 1.43                     | 0.83              |
| 23:BB:775:G:H4'    | 23:BB:776:G:H5'    | 1.59                     | 0.83              |
| 32:BK:108:ARG:NH2  | 37:BP:36:LYS:HG3   | 1.92                     | 0.83              |
| 42:BU:3:LYS:HB2    | 42:BU:3:LYS:NZ     | 1.90                     | 0.83              |
| 12:CM:38:ILE:HG13  | 12:CM:55:LEU:HD21  | 1.60                     | 0.83              |
| 23:DB:996:A:H5''   | 38:DQ:93:ILE:HG21  | 1.58                     | 0.83              |
| 34:DM:5:LYS:HE3    | 34:DM:6:ARG:H      | 1.43                     | 0.83              |
| 38:DQ:73:ILE:HG13  | 38:DQ:74:SER:H     | 1.43                     | 0.83              |
| 40:DS:25:ARG:HD2   | 40:DS:26:GLY:N     | 1.94                     | 0.83              |
| 1:AA:1005:A:H2'    | 1:AA:1006:G:O4'    | 1.78                     | 0.83              |
| 25:BC:42:ARG:HG2   | 25:BC:43:ASN:N     | 1.89                     | 0.83              |
| 4:CE:157:GLY:H     | 7:CH:43:GLY:HA3    | 1.41                     | 0.83              |
| 13:CN:96:LYS:HG2   | 13:CN:97:LYS:H     | 1.44                     | 0.83              |
| 31:DJ:84:ILE:HD12  | 31:DJ:85:LYS:N     | 1.92                     | 0.83              |
| 1:AA:781:A:H2'     | 1:AA:782:A:H5'     | 1.60                     | 0.83              |
| 23:BB:1024:G:H3'   | 23:BB:1025:G:H5''  | 1.59                     | 0.83              |
| 23:BB:2297:A:N6    | 23:BB:2319:G:H3'   | 1.93                     | 0.83              |
| 44:BX:35:GLY:HA3   | 44:BX:40:SER:HA    | 1.60                     | 0.83              |
| 39:DR:66:HIS:HA    | 39:DR:98:ILE:HD13  | 1.57                     | 0.83              |
| 20:CB:100:LEU:HB3  | 20:CB:178:LEU:HD11 | 1.61                     | 0.83              |
| 1:AA:967:C:H3'     | 1:AA:968:A:H5'     | 1.59                     | 0.83              |
| 3:AD:160:LEU:H     | 3:AD:160:LEU:HD13  | 1.44                     | 0.83              |
| 7:AH:5:PRO:HB2     | 7:AH:32:LYS:HZ1    | 1.41                     | 0.83              |
| 7:AH:5:PRO:HB2     | 7:AH:32:LYS:NZ     | 1.92                     | 0.83              |
| 23:BB:1060:U:C2    | 23:BB:1088:A:N7    | 2.47                     | 0.83              |
| 33:BL:84:LYS:HA    | 33:BL:84:LYS:NZ    | 1.93                     | 0.83              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:CE:36:THR:HG21  | 4:CE:63:MET:HG2    | 1.61                     | 0.83              |
| 23:DB:162:U:O2'   | 23:DB:163:C:H5'    | 1.79                     | 0.83              |
| 23:DB:2143:C:H2'  | 23:DB:2144:G:O4'   | 1.77                     | 0.83              |
| 23:DB:2309:A:H3'  | 23:DB:2310:C:H5''  | 1.60                     | 0.83              |
| 40:DS:23:LEU:HD13 | 40:DS:25:ARG:HH22  | 1.44                     | 0.83              |
| 42:DU:9:GLU:HB2   | 42:DU:71:ILE:HB    | 1.60                     | 0.83              |
| 1:AA:1320:C:H42   | 18:AS:35:ARG:HD3   | 1.43                     | 0.83              |
| 29:BG:27:GLY:HA3  | 29:BG:78:VAL:HB    | 1.60                     | 0.83              |
| 15:CP:3:THR:HG22  | 15:CP:66:THR:HB    | 1.61                     | 0.83              |
| 18:CS:32:THR:HG22 | 18:CS:33:TRP:H     | 1.43                     | 0.83              |
| 23:DB:775:G:H4'   | 23:DB:776:G:H5'    | 1.59                     | 0.83              |
| 23:BB:2845:U:O3'  | 37:BP:54:LEU:HG    | 1.78                     | 0.83              |
| 31:BJ:71:ASP:CG   | 31:BJ:72:LYS:H     | 1.85                     | 0.83              |
| 44:BX:14:LEU:HD21 | 44:BX:57:LEU:HB2   | 1.61                     | 0.83              |
| 19:CT:61:ALA:HA   | 19:CT:67:HIS:H     | 1.44                     | 0.83              |
| 41:DT:47:VAL:HG22 | 41:DT:53:VAL:HG21  | 1.61                     | 0.83              |
| 23:BB:1913:A:H1'  | 23:BB:1914:C:OP1   | 1.79                     | 0.82              |
| 27:BE:132:LYS:HZ2 | 27:BE:132:LYS:HB2  | 1.43                     | 0.82              |
| 44:BX:38:GLN:H    | 44:BX:38:GLN:NE2   | 1.75                     | 0.82              |
| 7:CH:11:THR:HG22  | 7:CH:14:ARG:HH12   | 1.44                     | 0.82              |
| 23:DB:136:G:C2    | 41:DT:3:ARG:CZ     | 2.62                     | 0.82              |
| 23:DB:1060:U:C2   | 23:DB:1088:A:N7    | 2.47                     | 0.82              |
| 9:AJ:8:ILE:HD12   | 9:AJ:100:ILE:HG22  | 1.61                     | 0.82              |
| 29:BG:173:ALA:C   | 29:BG:174:LYS:HD2  | 2.03                     | 0.82              |
| 18:CS:15:LEU:HA   | 18:CS:18:VAL:HG12  | 1.60                     | 0.82              |
| 23:DB:90:U:H3'    | 23:DB:91:A:H5''    | 1.59                     | 0.82              |
| 35:DN:41:ALA:HB1  | 35:DN:113:ILE:HD11 | 1.61                     | 0.82              |
| 23:BB:630:G:H1    | 33:BL:69:ARG:NH2   | 1.77                     | 0.82              |
| 25:BC:138:SER:HA  | 25:BC:162:GLN:HG2  | 1.61                     | 0.82              |
| 45:BY:9:THR:HB    | 45:BY:54:VAL:HA    | 1.58                     | 0.82              |
| 22:DA:30:C:H2'    | 22:DA:31:C:H5'     | 1.60                     | 0.82              |
| 35:DN:37:THR:HG22 | 35:DN:39:PRO:HD2   | 1.59                     | 0.82              |
| 35:DN:85:PRO:HA   | 35:DN:88:ALA:HB2   | 1.62                     | 0.82              |
| 23:BB:997:G:OP1   | 38:BQ:92:LYS:HD2   | 1.79                     | 0.82              |
| 45:BY:6:ILE:HG22  | 45:BY:56:VAL:HG23  | 1.62                     | 0.82              |
| 5:CF:99:ALA:HA    | 17:CR:23:LYS:HE2   | 1.62                     | 0.82              |
| 23:DB:7:G:H5'     | 31:DJ:134:ALA:O    | 1.80                     | 0.82              |
| 28:DF:64:PRO:HA   | 28:DF:88:VAL:HG22  | 1.61                     | 0.82              |
| 43:DW:3:LYS:HA    | 43:DW:3:LYS:NZ     | 1.94                     | 0.82              |
| 2:AC:78:LYS:HG2   | 2:AC:81:GLU:HB2    | 1.58                     | 0.82              |
| 12:AM:64:VAL:HA   | 12:AM:68:LEU:HD12  | 1.61                     | 0.82              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:742:A:H2'    | 23:DB:743:A:H8     | 1.43                     | 0.82              |
| 23:DB:1060:U:H5    | 52:DI:131:THR:HG22 | 1.43                     | 0.82              |
| 23:DB:2574:G:H21   | 26:DD:147:GLY:CA   | 1.92                     | 0.82              |
| 25:DC:139:THR:HA   | 25:DC:193:GLU:CD   | 2.05                     | 0.82              |
| 27:BE:88:ARG:HB2   | 27:BE:88:ARG:HH11  | 1.45                     | 0.82              |
| 23:DB:2334:U:H3    | 43:DW:74:LYS:HE2   | 1.44                     | 0.82              |
| 27:DE:142:ALA:H    | 27:DE:185:LYS:NZ   | 1.78                     | 0.82              |
| 36:DO:56:LYS:HE2   | 36:DO:81:ARG:NE    | 1.94                     | 0.82              |
| 23:BB:742:A:H2'    | 23:BB:743:A:H8     | 1.43                     | 0.82              |
| 23:BB:1639:C:C2'   | 23:BB:1640:A:H5''  | 2.09                     | 0.82              |
| 43:BW:27:GLY:HA2   | 43:BW:60:ALA:HA    | 1.60                     | 0.82              |
| 42:DU:13:LEU:H     | 42:DU:13:LEU:HD12  | 1.45                     | 0.82              |
| 52:DI:72:THR:HG21  | 52:DI:112:LYS:HA   | 1.62                     | 0.82              |
| 23:BB:287:G:H2'    | 23:BB:288:U:C6     | 2.15                     | 0.82              |
| 30:BH:128:HIS:HB3  | 30:BH:144:VAL:HB   | 1.61                     | 0.82              |
| 52:BI:55:PRO:HD3   | 52:BI:74:PRO:HD3   | 1.60                     | 0.82              |
| 23:DB:2336:A:H1'   | 23:DB:2337:G:OP1   | 1.79                     | 0.82              |
| 10:AK:83:VAL:HG23  | 10:AK:109:ILE:HA   | 1.60                     | 0.82              |
| 17:AR:52:ARG:HH11  | 17:AR:52:ARG:HB3   | 1.45                     | 0.82              |
| 33:BL:29:LYS:HD2   | 33:BL:31:GLY:N     | 1.95                     | 0.82              |
| 42:BU:7:ASP:H      | 42:BU:24:VAL:HA    | 1.45                     | 0.82              |
| 42:BU:25:LYS:HG3   | 42:BU:35:VAL:HA    | 1.62                     | 0.82              |
| 6:CG:129:ASN:HB3   | 6:CG:134:VAL:HG21  | 1.61                     | 0.82              |
| 10:CK:16:SER:HA    | 10:CK:78:ILE:HA    | 1.61                     | 0.82              |
| 52:DI:105:LEU:HD13 | 52:DI:129:GLU:HG2  | 1.61                     | 0.82              |
| 15:AP:12:LYS:HD2   | 15:AP:13:LYS:HE2   | 1.61                     | 0.82              |
| 23:BB:2297:A:H61   | 23:BB:2319:G:C3'   | 1.93                     | 0.82              |
| 33:BL:109:LYS:HA   | 33:BL:126:ARG:HA   | 1.62                     | 0.82              |
| 45:BY:7:THR:HA     | 45:BY:34:THR:HA    | 1.61                     | 0.82              |
| 30:DH:114:GLU:HB2  | 30:DH:133:GLN:HG3  | 1.60                     | 0.82              |
| 21:AU:20:ARG:HA    | 21:AU:24:LYS:HG3   | 1.59                     | 0.81              |
| 23:BB:2336:A:H1'   | 23:BB:2337:G:OP1   | 1.80                     | 0.81              |
| 34:BM:82:MET:HB2   | 34:BM:84:LYS:NZ    | 1.94                     | 0.81              |
| 23:DB:1639:C:C2'   | 23:DB:1640:A:H5''  | 2.09                     | 0.81              |
| 23:DB:2633:G:H1'   | 26:DD:62:LYS:HG3   | 1.61                     | 0.81              |
| 28:DF:96:TRP:O     | 28:DF:100:GLU:HG3  | 1.78                     | 0.81              |
| 18:AS:4:LEU:HD13   | 18:AS:9:PHE:H      | 1.45                     | 0.81              |
| 32:BK:35:VAL:HG23  | 32:BK:36:GLY:H     | 1.44                     | 0.81              |
| 36:BO:17:LYS:HE2   | 43:BW:77:LYS:HD2   | 1.61                     | 0.81              |
| 30:DH:122:LEU:HD13 | 30:DH:146:VAL:HG22 | 1.60                     | 0.81              |
| 42:DU:91:LYS:HD3   | 42:DU:93:ARG:HE    | 1.45                     | 0.81              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:AI:40:ARG:H      | 8:AI:44:ARG:HE     | 1.26                     | 0.81              |
| 8:AI:112:ARG:NH1   | 8:AI:112:ARG:HB2   | 1.95                     | 0.81              |
| 23:BB:340:A:H2'    | 23:BB:341:C:O4'    | 1.81                     | 0.81              |
| 30:BH:66:ASN:HA    | 30:BH:138:VAL:HG21 | 1.61                     | 0.81              |
| 36:BO:64:TYR:HE1   | 36:BO:74:VAL:HG11  | 1.46                     | 0.81              |
| 36:BO:87:ILE:HG13  | 36:BO:88:LYS:H     | 1.43                     | 0.81              |
| 23:DB:857:G:C2'    | 23:DB:858:G:H5'    | 2.10                     | 0.81              |
| 23:DB:1064:C:H4'   | 52:DI:90:GLY:HA2   | 1.60                     | 0.81              |
| 29:DG:171:LYS:HD3  | 29:DG:172:GLU:O    | 1.79                     | 0.81              |
| 33:DL:103:ILE:HG13 | 33:DL:104:GLN:H    | 1.45                     | 0.81              |
| 37:DP:28:LYS:HD3   | 37:DP:44:GLY:HA3   | 1.63                     | 0.81              |
| 3:AD:36:ALA:HA     | 3:AD:41:GLY:HA3    | 1.62                     | 0.81              |
| 23:BB:200:U:H5''   | 46:BZ:20:ASN:HB3   | 1.62                     | 0.81              |
| 23:BB:279:A:N6     | 23:BB:361:G:H1'    | 1.96                     | 0.81              |
| 28:BF:126:ASN:HD22 | 28:BF:126:ASN:N    | 1.78                     | 0.81              |
| 23:DB:899:A:H3'    | 23:DB:900:A:H8     | 1.45                     | 0.81              |
| 31:DJ:25:LEU:HD11  | 31:DJ:63:ALA:H     | 1.45                     | 0.81              |
| 39:DR:22:LEU:HD12  | 39:DR:24:LYS:H     | 1.43                     | 0.81              |
| 36:BO:8:ILE:HG22   | 36:BO:10:ARG:HG2   | 1.63                     | 0.81              |
| 42:BU:28:LEU:HB2   | 42:BU:31:GLY:HA3   | 1.61                     | 0.81              |
| 1:CA:1086:U:H3     | 1:CA:1099:G:H22    | 1.25                     | 0.81              |
| 20:CB:163:ILE:HG23 | 20:CB:164:ASP:H    | 1.46                     | 0.81              |
| 27:DE:99:LYS:C     | 27:DE:99:LYS:HZ2   | 1.87                     | 0.81              |
| 38:DQ:87:VAL:HB    | 39:DR:54:VAL:HG21  | 1.62                     | 0.81              |
| 43:DW:60:ALA:HB3   | 43:DW:80:SER:HA    | 1.63                     | 0.81              |
| 25:BC:163:ILE:HG22 | 25:BC:164:VAL:H    | 1.44                     | 0.81              |
| 31:BJ:100:VAL:HG22 | 31:BJ:101:ILE:H    | 1.45                     | 0.81              |
| 37:BP:47:ILE:HG22  | 37:BP:49:ILE:H     | 1.45                     | 0.81              |
| 37:BP:92:ARG:NH2   | 37:BP:110:LYS:HE2  | 1.95                     | 0.81              |
| 40:BS:71:VAL:HA    | 40:BS:106:VAL:O    | 1.80                     | 0.81              |
| 43:BW:42:THR:HB    | 43:BW:65:LYS:HA    | 1.60                     | 0.81              |
| 25:DC:172:THR:O    | 25:DC:173:LEU:HB2  | 1.81                     | 0.81              |
| 3:AD:194:ILE:HD13  | 3:AD:195:ASN:N     | 1.96                     | 0.81              |
| 9:AJ:87:LEU:HB3    | 9:AJ:88:MET:HE3    | 1.62                     | 0.81              |
| 11:AL:56:LEU:HD11  | 11:AL:81:ILE:HD12  | 1.61                     | 0.81              |
| 23:BB:1177:G:H2'   | 23:BB:1178:C:C6    | 2.16                     | 0.81              |
| 38:BQ:7:VAL:HG23   | 38:BQ:8:ILE:H      | 1.43                     | 0.81              |
| 23:DB:589:U:H4'    | 27:DE:87:ALA:HB2   | 1.61                     | 0.81              |
| 23:DB:2511:U:H5''  | 26:DD:129:THR:HG23 | 1.62                     | 0.81              |
| 12:AM:11:HIS:H     | 12:AM:44:ILE:HD11  | 1.44                     | 0.81              |
| 16:AQ:27:PHE:HB3   | 16:AQ:36:PHE:HB3   | 1.63                     | 0.81              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:BZ:26:SER:O     | 46:BZ:28:VAL:HG13  | 1.81                     | 0.81              |
| 3:CD:162:GLU:HG3   | 3:CD:163:GLN:HG3   | 1.63                     | 0.81              |
| 8:CI:45:MET:O      | 8:CI:49:GLN:HG3    | 1.80                     | 0.81              |
| 23:DB:250:G:H5'    | 50:D3:7:ARG:HG2    | 1.61                     | 0.81              |
| 52:DI:105:LEU:HD11 | 52:DI:139:VAL:HG21 | 1.62                     | 0.81              |
| 1:AA:238:A:H2'     | 1:AA:239:U:H5''    | 1.61                     | 0.81              |
| 38:BQ:73:ILE:HG23  | 38:BQ:77:LYS:HB2   | 1.62                     | 0.81              |
| 19:CT:45:ALA:HA    | 19:CT:48:LYS:HB3   | 1.63                     | 0.81              |
| 23:DB:458:G:N2     | 23:DB:469:G:H2'    | 1.95                     | 0.81              |
| 23:DB:717:C:H3'    | 23:DB:718:A:H5''   | 1.61                     | 0.81              |
| 25:DC:140:VAL:HA   | 25:DC:191:LEU:HA   | 1.62                     | 0.81              |
| 18:AS:5:LYS:HE3    | 18:AS:5:LYS:N      | 1.96                     | 0.81              |
| 31:BJ:16:TYR:HB2   | 31:BJ:54:ILE:HG22  | 1.63                     | 0.81              |
| 32:BK:64:ARG:H     | 32:BK:83:ALA:HB3   | 1.44                     | 0.81              |
| 27:DE:6:LYS:HD3    | 27:DE:7:ASP:H      | 1.46                     | 0.81              |
| 50:D3:7:ARG:NH1    | 50:D3:7:ARG:HA     | 1.95                     | 0.81              |
| 16:AQ:20:ILE:HG13  | 16:AQ:45:VAL:HB    | 1.61                     | 0.80              |
| 37:BP:25:VAL:HG13  | 37:BP:87:ARG:HA    | 1.61                     | 0.80              |
| 1:CA:1238:A:H5'    | 1:CA:1336:C:H41    | 1.45                     | 0.80              |
| 33:DL:39:LYS:H     | 33:DL:39:LYS:HZ3   | 1.26                     | 0.80              |
| 41:DT:34:VAL:HG21  | 41:DT:43:ILE:HD12  | 1.62                     | 0.80              |
| 46:DZ:59:ARG:HB3   | 46:DZ:63:ARG:HB2   | 1.61                     | 0.80              |
| 1:AA:1323:G:H2'    | 1:AA:1324:A:H8     | 1.44                     | 0.80              |
| 23:BB:580:U:O3'    | 38:BQ:30:VAL:HG13  | 1.80                     | 0.80              |
| 35:BN:96:ARG:HH21  | 35:BN:118:ARG:HB3  | 1.46                     | 0.80              |
| 23:DB:2377:A:N6    | 36:DO:13:ARG:HH21  | 1.78                     | 0.80              |
| 49:D2:35:ARG:HH22  | 49:D2:44:VAL:HG22  | 1.46                     | 0.80              |
| 2:AC:87:ARG:HG3    | 2:AC:100:ILE:HG22  | 1.63                     | 0.80              |
| 23:BB:265:A:O2'    | 23:BB:266:G:H4'    | 1.81                     | 0.80              |
| 25:BC:22:GLU:HA    | 25:BC:202:ARG:CZ   | 2.11                     | 0.80              |
| 26:BD:120:GLY:H    | 26:BD:123:LYS:HG3  | 1.43                     | 0.80              |
| 36:BO:1:MET:HG2    | 36:BO:3:LYS:H      | 1.45                     | 0.80              |
| 38:BQ:16:ILE:HD12  | 38:BQ:17:LEU:N     | 1.96                     | 0.80              |
| 39:BR:75:VAL:H     | 39:BR:90:ARG:NE    | 1.79                     | 0.80              |
| 33:DL:124:GLY:N    | 33:DL:142:ILE:HA   | 1.95                     | 0.80              |
| 38:DQ:87:VAL:HG12  | 38:DQ:89:ILE:HD13  | 1.62                     | 0.80              |
| 47:D0:27:LEU:H     | 47:D0:27:LEU:HD22  | 1.45                     | 0.80              |
| 23:BB:704:G:H2'    | 23:BB:726:G:H22    | 1.45                     | 0.80              |
| 23:BB:1568:G:OP1   | 25:BC:61:TYR:HB2   | 1.82                     | 0.80              |
| 25:BC:194:VAL:HG12 | 25:BC:195:GLY:H    | 1.45                     | 0.80              |
| 29:BG:153:PRO:HG2  | 29:BG:162:ARG:HB3  | 1.63                     | 0.80              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:238:A:H2'     | 1:CA:239:U:H5''   | 1.61                     | 0.80              |
| 23:DB:354:A:H2'    | 23:DB:355:U:C6    | 2.17                     | 0.80              |
| 30:DH:115:VAL:HG22 | 30:DH:117:LEU:H   | 1.45                     | 0.80              |
| 32:DK:2:ILE:HD13   | 32:DK:6:THR:HG21  | 1.61                     | 0.80              |
| 33:DL:7:SER:CB     | 33:DL:8:PRO:HD3   | 2.07                     | 0.80              |
| 37:DP:50:ARG:NH1   | 37:DP:50:ARG:HB2  | 1.97                     | 0.80              |
| 3:AD:84:ASN:ND2    | 3:AD:87:GLU:H     | 1.79                     | 0.80              |
| 8:AI:35:GLU:HA     | 8:AI:39:GLY:HA3   | 1.64                     | 0.80              |
| 23:BB:1178:C:H2'   | 23:BB:1179:G:C8   | 2.16                     | 0.80              |
| 31:BJ:35:ARG:HE    | 31:BJ:39:LYS:HB3  | 1.46                     | 0.80              |
| 29:DG:40:VAL:HG22  | 29:DG:51:PHE:HE2  | 1.44                     | 0.80              |
| 39:DR:64:VAL:HG22  | 39:DR:65:ALA:H    | 1.46                     | 0.80              |
| 2:AC:176:THR:HB    | 2:AC:179:ALA:HB2  | 1.63                     | 0.80              |
| 3:AD:94:GLU:HG3    | 3:AD:103:ARG:HH12 | 1.46                     | 0.80              |
| 43:BW:36:ILE:HD12  | 43:BW:69:GLU:OE2  | 1.82                     | 0.80              |
| 1:CA:1451:U:H5''   | 1:CA:1452:C:OP2   | 1.81                     | 0.80              |
| 32:DK:78:ARG:HH22  | 37:DP:62:LYS:NZ   | 1.80                     | 0.80              |
| 1:AA:1201:A:H1'    | 1:AA:1202:U:OP2   | 1.81                     | 0.80              |
| 23:DB:1007:C:H5''  | 31:DJ:37:ARG:HH12 | 1.47                     | 0.80              |
| 37:DP:69:VAL:HG13  | 37:DP:70:GLU:H    | 1.45                     | 0.80              |
| 1:AA:1026:G:H2'    | 1:AA:1027:C:H6    | 1.47                     | 0.80              |
| 23:BB:144:A:H2'    | 23:BB:145:C:H6    | 1.47                     | 0.80              |
| 31:BJ:25:LEU:HD12  | 31:BJ:62:VAL:HA   | 1.63                     | 0.80              |
| 39:BR:4:VAL:HA     | 39:BR:12:HIS:HB3  | 1.63                     | 0.80              |
| 41:BT:12:ARG:HH21  | 44:BX:29:ARG:HH12 | 1.27                     | 0.80              |
| 6:CG:112:ASP:HB2   | 6:CG:118:ARG:HG2  | 1.62                     | 0.80              |
| 26:DD:37:VAL:HG13  | 26:DD:42:ASN:HB3  | 1.63                     | 0.80              |
| 27:DE:152:GLU:HA   | 27:DE:188:MET:HE2 | 1.64                     | 0.80              |
| 28:DF:98:PHE:HA    | 28:DF:101:ARG:HE  | 1.45                     | 0.80              |
| 31:DJ:121:LYS:HE3  | 31:DJ:121:LYS:N   | 1.97                     | 0.80              |
| 33:DL:135:ILE:HG22 | 33:DL:138:ALA:HB3 | 1.63                     | 0.80              |
| 1:AA:946:A:H2'     | 1:AA:947:G:C8     | 2.16                     | 0.80              |
| 20:AB:96:LEU:H     | 20:AB:99:MET:HE3  | 1.46                     | 0.80              |
| 39:BR:6:GLN:HA     | 39:BR:10:LYS:HA   | 1.64                     | 0.80              |
| 39:BR:58:VAL:HG13  | 39:BR:59:ILE:HG12 | 1.61                     | 0.80              |
| 52:BI:106:GLN:O    | 52:BI:110:GLN:HG3 | 1.81                     | 0.80              |
| 4:CE:36:THR:HG22   | 4:CE:37:VAL:H     | 1.46                     | 0.80              |
| 27:DE:120:VAL:HG12 | 27:DE:121:VAL:H   | 1.45                     | 0.80              |
| 30:DH:31:VAL:HA    | 30:DH:36:ALA:HA   | 1.63                     | 0.80              |
| 31:DJ:25:LEU:HG    | 31:DJ:64:VAL:H    | 1.47                     | 0.80              |
| 1:AA:1326:U:H2'    | 1:AA:1327:C:H6    | 1.47                     | 0.80              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:100:U:H4'    | 42:BU:90:LYS:CE    | 2.12                     | 0.80              |
| 25:BC:88:ALA:HB1   | 25:BC:156:SER:HB3  | 1.64                     | 0.80              |
| 32:BK:88:ASN:ND2   | 32:BK:91:SER:HB2   | 1.97                     | 0.80              |
| 33:BL:60:ARG:HA    | 50:B3:11:LYS:HE2   | 1.63                     | 0.80              |
| 40:BS:50:VAL:HG11  | 40:BS:103:ILE:HG21 | 1.62                     | 0.80              |
| 10:CK:70:ALA:HB1   | 10:CK:74:LYS:HD2   | 1.64                     | 0.80              |
| 21:CU:14:ALA:HB3   | 21:CU:16:ARG:NH1   | 1.97                     | 0.80              |
| 26:DD:109:VAL:HG11 | 26:DD:193:VAL:HG12 | 1.64                     | 0.80              |
| 33:DL:109:LYS:HG2  | 33:DL:126:ARG:HD3  | 1.63                     | 0.80              |
| 37:DP:64:SER:HA    | 37:DP:71:ARG:HB2   | 1.62                     | 0.80              |
| 23:BB:279:A:C2     | 23:BB:362:A:H4'    | 2.17                     | 0.79              |
| 23:BB:692:C:C5'    | 25:BC:42:ARG:HB2   | 2.12                     | 0.79              |
| 23:BB:1131:G:H1'   | 23:BB:1133:A:H62   | 1.47                     | 0.79              |
| 31:BJ:25:LEU:HG    | 31:BJ:64:VAL:H     | 1.47                     | 0.79              |
| 31:BJ:72:LYS:HB2   | 31:BJ:90:GLU:HB2   | 1.61                     | 0.79              |
| 41:BT:1:MET:SD     | 41:BT:2:ILE:HG12   | 2.21                     | 0.79              |
| 14:CO:55:LEU:HA    | 14:CO:58:MET:HE3   | 1.63                     | 0.79              |
| 23:DB:1098:A:H3'   | 52:DI:3:LYS:CB     | 2.11                     | 0.79              |
| 38:DQ:69:ARG:HH11  | 38:DQ:69:ARG:HB3   | 1.47                     | 0.79              |
| 45:DY:10:ARG:HA    | 45:DY:31:ILE:HD12  | 1.64                     | 0.79              |
| 48:D1:12:SER:HA    | 48:D1:50:GLU:HA    | 1.63                     | 0.79              |
| 8:AI:110:VAL:HG12  | 8:AI:111:GLU:H     | 1.45                     | 0.79              |
| 23:BB:162:U:H4'    | 23:BB:163:C:OP1    | 1.82                     | 0.79              |
| 27:BE:153:LEU:HD13 | 27:BE:193:VAL:HG21 | 1.65                     | 0.79              |
| 33:BL:84:LYS:HA    | 33:BL:84:LYS:HZ2   | 1.45                     | 0.79              |
| 39:BR:41:ILE:O     | 39:BR:41:ILE:HD12  | 1.83                     | 0.79              |
| 4:CE:33:THR:HG22   | 4:CE:51:LYS:HG2    | 1.64                     | 0.79              |
| 37:DP:25:VAL:HG13  | 37:DP:88:ARG:H     | 1.46                     | 0.79              |
| 52:DI:21:PRO:HB2   | 52:DI:22:PRO:HD3   | 1.64                     | 0.79              |
| 5:AF:88:MET:HE1    | 5:AF:90:MET:HG3    | 1.64                     | 0.79              |
| 26:BD:4:LEU:HD13   | 26:BD:79:LEU:HD11  | 1.65                     | 0.79              |
| 30:BH:83:LYS:HB3   | 30:BH:91:PHE:HD1   | 1.43                     | 0.79              |
| 34:BM:42:THR:HA    | 34:BM:92:TRP:CD1   | 2.16                     | 0.79              |
| 37:BP:2:ASN:H      | 37:BP:2:ASN:HD22   | 1.30                     | 0.79              |
| 2:CC:18:ASN:HA     | 2:CC:55:VAL:HG12   | 1.65                     | 0.79              |
| 23:DB:85:G:H5'     | 42:DU:28:LEU:HB3   | 1.61                     | 0.79              |
| 41:BT:12:ARG:HH21  | 44:BX:29:ARG:NH1   | 1.80                     | 0.79              |
| 1:CA:60:A:H2'      | 19:CT:4:LYS:HE3    | 1.64                     | 0.79              |
| 23:DB:1176:U:H2'   | 23:DB:1177:G:C8    | 2.17                     | 0.79              |
| 28:DF:140:ILE:HG22 | 28:DF:142:TYR:H    | 1.47                     | 0.79              |
| 33:DL:81:ASP:HA    | 33:DL:84:LYS:HD3   | 1.64                     | 0.79              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:972:A:H3'    | 23:BB:973:A:H5''   | 1.63                     | 0.79              |
| 41:BT:8:LEU:HA     | 44:BX:19:LEU:HD21  | 1.64                     | 0.79              |
| 2:CC:120:THR:HG23  | 2:CC:188:ALA:HB2   | 1.63                     | 0.79              |
| 23:DB:320:A:H4'    | 23:DB:322:A:N7     | 1.97                     | 0.79              |
| 23:DB:1006:C:H5''  | 31:DJ:34:ARG:HE    | 1.48                     | 0.79              |
| 28:DF:133:GLU:N    | 28:DF:150:GLY:HA2  | 1.98                     | 0.79              |
| 30:DH:114:GLU:HB3  | 30:DH:133:GLN:HE21 | 1.47                     | 0.79              |
| 47:D0:53:VAL:HG13  | 47:D0:54:ILE:HG13  | 1.65                     | 0.79              |
| 23:BB:1197:G:H2'   | 23:BB:1198:U:C6    | 2.18                     | 0.79              |
| 23:BB:1813:G:H21   | 25:BC:51:ARG:HG2   | 1.46                     | 0.79              |
| 25:BC:50:THR:HG22  | 25:BC:51:ARG:HG3   | 1.65                     | 0.79              |
| 33:BL:38:GLN:CD    | 33:BL:39:LYS:H     | 1.89                     | 0.79              |
| 1:CA:1003:G:N2     | 1:CA:1005:A:H5'    | 1.97                     | 0.79              |
| 1:CA:1311:A:H62    | 18:CS:1:PRO:HD3    | 1.48                     | 0.79              |
| 4:CE:158:LYS:HB3   | 7:CH:63:LYS:HD3    | 1.65                     | 0.79              |
| 13:CN:63:CYS:HB3   | 13:CN:68:ARG:H     | 1.47                     | 0.79              |
| 20:CB:202:ASN:ND2  | 20:CB:203:ASP:H    | 1.79                     | 0.79              |
| 22:DA:48:U:H2'     | 22:DA:49:C:H6      | 1.44                     | 0.79              |
| 41:DT:56:GLU:O     | 41:DT:57:VAL:HG22  | 1.82                     | 0.79              |
| 30:BH:3:VAL:HB     | 30:BH:37:VAL:HB    | 1.64                     | 0.79              |
| 6:CG:23:ALA:O      | 6:CG:26:VAL:HG22   | 1.82                     | 0.79              |
| 8:CI:17:ARG:HB3    | 8:CI:65:THR:HB     | 1.65                     | 0.79              |
| 24:DV:70:ILE:HD12  | 24:DV:71:LYS:H     | 1.47                     | 0.79              |
| 25:DC:63:ILE:HG21  | 25:DC:90:ILE:HD11  | 1.64                     | 0.79              |
| 27:DE:53:THR:HB    | 27:DE:74:LYS:HG2   | 1.63                     | 0.79              |
| 33:DL:44:GLY:HA2   | 33:DL:47:ARG:HE    | 1.46                     | 0.79              |
| 45:DY:45:GLY:HA2   | 45:DY:48:ASN:HD22  | 1.46                     | 0.79              |
| 22:BA:49:C:H2'     | 22:BA:50:A:H8      | 1.48                     | 0.79              |
| 23:BB:3:U:HO2'     | 23:BB:4:U:H6       | 1.29                     | 0.79              |
| 23:BB:37:C:H2'     | 27:BE:46:GLN:HG2   | 1.63                     | 0.79              |
| 25:BC:3:VAL:HG12   | 25:BC:4:LYS:H      | 1.48                     | 0.79              |
| 25:BC:128:THR:HA   | 25:BC:190:THR:HA   | 1.62                     | 0.79              |
| 26:BD:11:MET:HG2   | 26:BD:12:THR:H     | 1.45                     | 0.79              |
| 27:BE:118:LEU:HD23 | 27:BE:118:LEU:H    | 1.45                     | 0.79              |
| 33:BL:61:LEU:CB    | 33:BL:62:PRO:HD2   | 2.12                     | 0.79              |
| 13:CN:50:LEU:H     | 13:CN:51:PRO:CD    | 1.95                     | 0.79              |
| 16:CQ:66:LEU:H     | 16:CQ:66:LEU:HD12  | 1.47                     | 0.79              |
| 28:DF:35:LEU:HB3   | 28:DF:151:LEU:HD11 | 1.64                     | 0.79              |
| 34:DM:4:PRO:HD2    | 34:DM:43:ALA:HB1   | 1.65                     | 0.79              |
| 44:DX:4:LYS:O      | 44:DX:7:ARG:HG2    | 1.82                     | 0.79              |
| 52:DI:11:GLN:HG2   | 52:DI:55:PRO:HB3   | 1.64                     | 0.79              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:17:U:H2'      | 1:AA:18:C:C6       | 2.18                     | 0.79              |
| 5:AF:53:LYS:HZ3    | 5:AF:53:LYS:HA     | 1.48                     | 0.79              |
| 8:AI:56:MET:HA     | 8:AI:59:LYS:HZ2    | 1.48                     | 0.79              |
| 9:AJ:40:ILE:HG13   | 9:AJ:73:LEU:HB3    | 1.65                     | 0.79              |
| 16:AQ:10:ARG:CZ    | 16:AQ:11:VAL:H     | 1.95                     | 0.79              |
| 31:BJ:39:LYS:HZ1   | 38:BQ:69:ARG:HD2   | 1.46                     | 0.79              |
| 33:BL:27:LEU:H     | 33:BL:27:LEU:HD12  | 1.47                     | 0.79              |
| 34:BM:41:LEU:HB2   | 34:BM:93:VAL:HG22  | 1.64                     | 0.79              |
| 52:BI:27:LEU:HD12  | 52:BI:32:VAL:HG11  | 1.64                     | 0.79              |
| 2:CC:137:VAL:HA    | 2:CC:148:ILE:HD13  | 1.63                     | 0.79              |
| 5:CF:47:LEU:HD13   | 5:CF:51:ILE:HG22   | 1.62                     | 0.79              |
| 33:DL:4:ASN:O      | 33:DL:6:LEU:HD22   | 1.82                     | 0.79              |
| 9:AJ:88:MET:HB2    | 9:AJ:89:ARG:HH12   | 1.47                     | 0.79              |
| 27:BE:113:VAL:HG23 | 27:BE:117:ARG:CZ   | 2.13                     | 0.79              |
| 34:BM:126:ILE:HG13 | 34:BM:127:LYS:H    | 1.47                     | 0.79              |
| 51:B4:2:LYS:HG2    | 51:B4:36:ARG:HB3   | 1.64                     | 0.79              |
| 1:CA:946:A:H2'     | 1:CA:947:G:C8      | 2.18                     | 0.79              |
| 23:DB:1099:G:H5''  | 52:DI:3:LYS:N      | 1.98                     | 0.79              |
| 23:DB:2800:A:H2'   | 23:DB:2801:G:O4'   | 1.83                     | 0.79              |
| 29:DG:120:ILE:HG12 | 29:DG:134:GLY:HA3  | 1.65                     | 0.79              |
| 30:DH:68:ARG:HE    | 30:DH:71:LYS:HE2   | 1.47                     | 0.79              |
| 35:DN:8:ARG:HD2    | 35:DN:46:ARG:NE    | 1.98                     | 0.79              |
| 46:DZ:66:ILE:HB    | 46:DZ:67:PRO:HD3   | 1.64                     | 0.79              |
| 1:AA:436:C:O2'     | 1:AA:437:U:H5'     | 1.83                     | 0.78              |
| 6:AG:4:ARG:HE      | 6:AG:5:VAL:H       | 1.30                     | 0.78              |
| 23:BB:86:G:OP1     | 42:BU:29:SER:HB2   | 1.83                     | 0.78              |
| 43:BW:28:GLU:HB3   | 43:BW:30:VAL:HG23  | 1.65                     | 0.78              |
| 46:BZ:44:PHE:HD1   | 46:BZ:44:PHE:H     | 1.30                     | 0.78              |
| 23:DB:1802:A:H4'   | 25:DC:255:LYS:HE2  | 1.63                     | 0.78              |
| 25:BC:140:VAL:O    | 25:BC:193:GLU:HB2  | 1.82                     | 0.78              |
| 26:BD:37:VAL:HG22  | 26:BD:46:ARG:HE    | 1.48                     | 0.78              |
| 37:BP:108:ARG:HD2  | 37:BP:108:ARG:H    | 1.48                     | 0.78              |
| 43:BW:66:VAL:HG13  | 43:BW:67:LYS:H     | 1.47                     | 0.78              |
| 23:DB:2309:A:H5'   | 23:DB:2310:C:OP2   | 1.83                     | 0.78              |
| 37:DP:30:TRP:HB2   | 37:DP:83:ILE:HB    | 1.64                     | 0.78              |
| 13:AN:65:GLN:HB2   | 13:AN:78:LEU:HD22  | 1.63                     | 0.78              |
| 23:BB:222:A:H61    | 23:BB:232:G:H1'    | 1.45                     | 0.78              |
| 23:BB:2216:G:H2'   | 23:BB:2217:G:H8    | 1.47                     | 0.78              |
| 23:BB:2511:U:H4'   | 26:BD:128:ARG:CZ   | 2.13                     | 0.78              |
| 23:BB:2800:A:H2'   | 23:BB:2801:G:O4'   | 1.84                     | 0.78              |
| 30:BH:68:ARG:HG3   | 30:BH:134:VAL:HG11 | 1.65                     | 0.78              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:BL:60:ARG:HD2   | 50:B3:7:ARG:NE     | 1.98                     | 0.78              |
| 42:BU:35:VAL:HG12  | 42:BU:36:GLU:H     | 1.47                     | 0.78              |
| 23:DB:922:C:H1'    | 43:DW:22:VAL:HG21  | 1.66                     | 0.78              |
| 23:DB:1080:A:H2'   | 23:DB:1081:U:H6    | 1.45                     | 0.78              |
| 39:DR:40:MET:HG2   | 39:DR:54:VAL:HG13  | 1.65                     | 0.78              |
| 1:AA:79:G:H2'      | 1:AA:80:A:C8       | 2.19                     | 0.78              |
| 1:AA:562:U:H1'     | 11:AL:11:ARG:HB3   | 1.65                     | 0.78              |
| 10:AK:92:ARG:HH11  | 10:AK:92:ARG:HB3   | 1.48                     | 0.78              |
| 23:BB:328:U:H4'    | 42:BU:65:GLN:HG3   | 1.65                     | 0.78              |
| 23:BB:597:G:H4'    | 33:BL:21:ARG:HE    | 1.48                     | 0.78              |
| 34:BM:67:VAL:HB    | 34:BM:100:LYS:HG2  | 1.63                     | 0.78              |
| 36:BO:37:ALA:O     | 36:BO:38:GLN:HG2   | 1.84                     | 0.78              |
| 48:B1:12:SER:HA    | 48:B1:50:GLU:HB3   | 1.64                     | 0.78              |
| 13:CN:40:ARG:HH12  | 18:CS:5:LYS:HB2    | 1.48                     | 0.78              |
| 27:DE:137:LYS:HA   | 27:DE:137:LYS:NZ   | 1.98                     | 0.78              |
| 35:DN:48:VAL:HA    | 35:DN:51:LEU:HD12  | 1.66                     | 0.78              |
| 43:DW:66:VAL:HG13  | 43:DW:67:LYS:H     | 1.47                     | 0.78              |
| 52:DI:45:THR:HA    | 52:DI:48:ILE:HG22  | 1.64                     | 0.78              |
| 45:BY:16:LEU:HB2   | 45:BY:17:PRO:CD    | 2.14                     | 0.78              |
| 23:DB:365:U:H2'    | 23:DB:366:C:C6     | 2.18                     | 0.78              |
| 23:DB:1098:A:H2'   | 52:DI:3:LYS:C      | 2.08                     | 0.78              |
| 26:DD:89:GLU:HG2   | 26:DD:93:GLY:HA3   | 1.64                     | 0.78              |
| 26:DD:170:VAL:HB   | 26:DD:194:PRO:HG2  | 1.66                     | 0.78              |
| 37:DP:29:VAL:HG21  | 37:DP:61:ARG:HH22  | 1.48                     | 0.78              |
| 3:AD:123:MET:HA    | 3:AD:128:VAL:HA    | 1.65                     | 0.78              |
| 23:BB:146:A:H2'    | 23:BB:147:C:C6     | 2.19                     | 0.78              |
| 34:BM:108:VAL:HG23 | 34:BM:112:LEU:HD11 | 1.65                     | 0.78              |
| 3:AD:118:SER:HA    | 3:AD:130:ASN:HB2   | 1.65                     | 0.78              |
| 3:AD:159:GLU:HG3   | 3:AD:160:LEU:N     | 1.96                     | 0.78              |
| 27:BE:122:GLU:HB3  | 27:BE:152:GLU:HB2  | 1.65                     | 0.78              |
| 5:CF:4:TYR:HA      | 5:CF:91:ARG:HA     | 1.64                     | 0.78              |
| 8:CI:18:VAL:HG12   | 8:CI:64:ILE:HA     | 1.64                     | 0.78              |
| 34:DM:15:GLY:O     | 34:DM:16:ARG:HG3   | 1.83                     | 0.78              |
| 34:DM:134:THR:HG22 | 34:DM:135:VAL:H    | 1.46                     | 0.78              |
| 51:D4:26:ILE:O     | 51:D4:27:CYS:HB2   | 1.83                     | 0.78              |
| 13:AN:60:ARG:HE    | 13:AN:62:ARG:NE    | 1.82                     | 0.78              |
| 23:BB:483:A:H5'    | 42:BU:43:LYS:HE2   | 1.66                     | 0.78              |
| 23:BB:1283:G:N2    | 23:BB:1286:A:H5'   | 1.98                     | 0.78              |
| 30:BH:37:VAL:N     | 30:BH:38:PRO:HD2   | 1.95                     | 0.78              |
| 34:BM:40:ARG:HH11  | 34:BM:92:TRP:HE3   | 1.29                     | 0.78              |
| 43:BW:32:ALA:O     | 43:BW:66:VAL:HG11  | 1.84                     | 0.78              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:BI:25:PRO:O     | 52:BI:29:GLN:HG2   | 1.84                     | 0.78              |
| 10:CK:82:GLU:HB3   | 10:CK:108:ASN:HD22 | 1.48                     | 0.78              |
| 21:CU:41:THR:HA    | 21:CU:45:LYS:HD3   | 1.65                     | 0.78              |
| 24:DV:9:ARG:HG2    | 24:DV:41:GLU:HG2   | 1.66                     | 0.78              |
| 37:DP:25:VAL:HG12  | 37:DP:27:VAL:H     | 1.47                     | 0.78              |
| 45:DY:18:LYS:HD2   | 45:DY:18:LYS:N     | 1.99                     | 0.78              |
| 23:BB:414:C:H2'    | 23:BB:415:A:H8     | 1.49                     | 0.78              |
| 23:BB:2674:G:H4'   | 32:BK:30:ARG:HG2   | 1.66                     | 0.78              |
| 25:BC:21:PRO:HG2   | 25:BC:202:ARG:HH11 | 1.48                     | 0.78              |
| 42:BU:39:ASN:ND2   | 42:BU:42:LYS:HE2   | 1.99                     | 0.78              |
| 9:CJ:40:ILE:HD11   | 9:CJ:73:LEU:HD12   | 1.65                     | 0.78              |
| 23:DB:2511:U:H5''  | 26:DD:129:THR:CG2  | 2.14                     | 0.78              |
| 28:DF:134:GLN:HB3  | 28:DF:136:ILE:HG13 | 1.65                     | 0.78              |
| 31:DJ:41:LYS:NZ    | 38:DQ:63:ARG:HD2   | 1.99                     | 0.78              |
| 35:DN:86:ARG:HH11  | 35:DN:86:ARG:HB3   | 1.47                     | 0.78              |
| 12:AM:19:THR:HA    | 12:AM:24:VAL:HG23  | 1.65                     | 0.78              |
| 20:AB:36:LYS:HE3   | 20:AB:36:LYS:N     | 1.98                     | 0.78              |
| 23:BB:2867:G:H2'   | 23:BB:2867:G:N3    | 1.98                     | 0.78              |
| 31:BJ:81:ILE:HG13  | 31:BJ:82:GLY:N     | 1.99                     | 0.78              |
| 1:CA:17:U:H2'      | 1:CA:18:C:C6       | 2.19                     | 0.78              |
| 1:CA:436:C:O2'     | 1:CA:437:U:H5'     | 1.83                     | 0.78              |
| 5:CF:62:MET:HG3    | 5:CF:64:VAL:HG23   | 1.66                     | 0.78              |
| 45:DY:4:ILE:N      | 45:DY:36:GLU:HG3   | 1.99                     | 0.78              |
| 50:D3:7:ARG:HA     | 50:D3:7:ARG:HH11   | 1.49                     | 0.78              |
| 18:AS:39:ILE:HG21  | 18:AS:65:MET:HB3   | 1.63                     | 0.77              |
| 25:BC:127:ASN:ND2  | 25:BC:128:THR:H    | 1.82                     | 0.77              |
| 38:BQ:33:VAL:HG23  | 38:BQ:37:ALA:HB3   | 1.66                     | 0.77              |
| 34:DM:117:PHE:HB2  | 34:DM:124:LEU:HD11 | 1.67                     | 0.77              |
| 12:AM:23:GLY:HA3   | 12:AM:64:VAL:HG13  | 1.64                     | 0.77              |
| 16:AQ:80:LYS:O     | 16:AQ:80:LYS:HE3   | 1.84                     | 0.77              |
| 20:AB:58:LYS:HG2   | 20:AB:62:ARG:HH21  | 1.50                     | 0.77              |
| 23:BB:663:G:H5''   | 33:BL:25:SER:HB2   | 1.64                     | 0.77              |
| 1:CA:975:A:O2'     | 1:CA:1358:U:H1'    | 1.84                     | 0.77              |
| 26:DD:77:ARG:NH1   | 26:DD:77:ARG:HB2   | 1.98                     | 0.77              |
| 20:AB:67:LEU:HD12  | 20:AB:153:MET:HE2  | 1.65                     | 0.77              |
| 23:BB:918:A:H2'    | 23:BB:919:U:H5'    | 1.66                     | 0.77              |
| 35:BN:116:VAL:HG22 | 35:BN:117:ASP:H    | 1.49                     | 0.77              |
| 36:BO:38:GLN:HA    | 36:BO:50:ALA:HB3   | 1.67                     | 0.77              |
| 37:BP:25:VAL:HG12  | 37:BP:27:VAL:HG12  | 1.67                     | 0.77              |
| 16:CQ:13:SER:HB3   | 16:CQ:21:VAL:HB    | 1.66                     | 0.77              |
| 25:DC:229:HIS:ND1  | 25:DC:230:PRO:HD2  | 1.99                     | 0.77              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:DD:8:LYS:HE2    | 37:DP:5:LYS:HG3    | 1.67                     | 0.77              |
| 29:DG:151:ARG:HB2  | 29:DG:151:ARG:HH11 | 1.47                     | 0.77              |
| 37:DP:90:ALA:H     | 37:DP:112:ARG:HH21 | 1.32                     | 0.77              |
| 26:BD:106:LYS:HA   | 26:BD:176:ASP:HA   | 1.66                     | 0.77              |
| 43:BW:43:LYS:HG2   | 43:BW:76:ARG:HH21  | 1.49                     | 0.77              |
| 10:CK:23:HIS:HB3   | 10:CK:30:ILE:HG13  | 1.65                     | 0.77              |
| 18:CS:27:LYS:HG3   | 18:CS:28:LYS:HD2   | 1.65                     | 0.77              |
| 27:DE:50:ALA:O     | 27:DE:74:LYS:HD3   | 1.83                     | 0.77              |
| 28:DF:174:PHE:H    | 28:DF:175:PRO:HD2  | 1.49                     | 0.77              |
| 32:DK:76:VAL:HB    | 37:DP:74:GLN:HE21  | 1.50                     | 0.77              |
| 1:AA:430:A:OP1     | 3:AD:8:LEU:HB2     | 1.84                     | 0.77              |
| 18:AS:20:LYS:HB3   | 18:AS:20:LYS:HZ2   | 1.49                     | 0.77              |
| 23:BB:2578:G:H1'   | 26:BD:145:SER:OG   | 1.83                     | 0.77              |
| 31:BJ:58:ASN:ND2   | 31:BJ:128:ASN:HB2  | 1.99                     | 0.77              |
| 31:BJ:61:LYS:HE2   | 31:BJ:61:LYS:HA    | 1.64                     | 0.77              |
| 34:BM:20:LEU:HD13  | 34:BM:38:ARG:HG2   | 1.66                     | 0.77              |
| 13:CN:26:LEU:HA    | 13:CN:29:ILE:HD12  | 1.65                     | 0.77              |
| 19:CT:69:ASN:ND2   | 19:CT:69:ASN:H     | 1.82                     | 0.77              |
| 23:DB:1283:G:N2    | 23:DB:1286:A:H5'   | 1.98                     | 0.77              |
| 23:BB:2576:G:OP2   | 26:BD:149:ASN:HB2  | 1.84                     | 0.77              |
| 28:BF:126:ASN:HD22 | 28:BF:126:ASN:H    | 1.30                     | 0.77              |
| 38:BQ:94:LEU:HD13  | 38:BQ:94:LEU:H     | 1.49                     | 0.77              |
| 51:B4:23:ILE:HG13  | 51:B4:35:GLN:HB3   | 1.65                     | 0.77              |
| 23:DB:966:G:H5'    | 23:DB:2272:U:O2    | 1.84                     | 0.77              |
| 23:DB:2867:G:H2'   | 23:DB:2867:G:N3    | 1.98                     | 0.77              |
| 8:AI:11:ARG:HH21   | 8:AI:12:LYS:HB2    | 1.49                     | 0.77              |
| 30:BH:81:ALA:HA    | 30:BH:146:VAL:HA   | 1.66                     | 0.77              |
| 34:BM:71:LYS:HD3   | 34:BM:92:TRP:C     | 2.09                     | 0.77              |
| 34:BM:100:LYS:HE3  | 34:BM:100:LYS:H    | 1.49                     | 0.77              |
| 39:DR:60:LYS:O     | 39:DR:60:LYS:HD3   | 1.85                     | 0.77              |
| 41:DT:38:ALA:HB1   | 41:DT:43:ILE:HD11  | 1.65                     | 0.77              |
| 52:DI:27:LEU:HD12  | 52:DI:32:VAL:HG11  | 1.66                     | 0.77              |
| 1:AA:1412:C:H2'    | 1:AA:1413:A:C8     | 2.20                     | 0.77              |
| 2:AC:58:ARG:HG2    | 2:AC:63:ILE:HG22   | 1.67                     | 0.77              |
| 23:BB:2008:C:H2'   | 23:BB:2009:A:H8    | 1.50                     | 0.77              |
| 26:BD:13:ARG:HA    | 26:BD:13:ARG:NH1   | 2.00                     | 0.77              |
| 26:BD:62:LYS:HG2   | 26:BD:63:PRO:HD3   | 1.65                     | 0.77              |
| 35:BN:100:CYS:HB3  | 35:BN:110:MET:HB2  | 1.66                     | 0.77              |
| 23:DB:2293:G:H5''  | 36:DO:9:ARG:NH2    | 1.99                     | 0.77              |
| 45:DY:45:GLY:HA2   | 45:DY:48:ASN:ND2   | 2.00                     | 0.77              |
| 5:AF:10:VAL:HA     | 5:AF:84:VAL:HA     | 1.67                     | 0.77              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:2064:C:H2'   | 23:BB:2065:C:C6    | 2.19                     | 0.77              |
| 30:BH:73:ASN:ND2   | 30:BH:74:ALA:H     | 1.82                     | 0.77              |
| 49:B2:12:ARG:HH21  | 49:B2:18:PHE:H     | 1.31                     | 0.77              |
| 33:DL:39:LYS:HZ3   | 33:DL:39:LYS:N     | 1.83                     | 0.77              |
| 23:BB:441:U:O2'    | 23:BB:442:G:H5'    | 1.84                     | 0.77              |
| 23:BB:2324:U:H5'   | 23:BB:2325:G:H5''  | 1.67                     | 0.77              |
| 25:BC:153:LEU:HD23 | 25:BC:153:LEU:H    | 1.49                     | 0.77              |
| 31:BJ:57:LEU:HB3   | 31:BJ:128:ASN:HA   | 1.66                     | 0.77              |
| 52:BI:21:PRO:HB2   | 52:BI:22:PRO:HD3   | 1.66                     | 0.77              |
| 23:DB:51:G:O2'     | 23:DB:118:A:N6     | 2.17                     | 0.77              |
| 1:AA:1461:G:H2'    | 1:AA:1462:C:C6     | 2.20                     | 0.76              |
| 40:BS:90:LYS:N     | 40:BS:90:LYS:HZ3   | 1.82                     | 0.76              |
| 50:B3:48:MET:SD    | 50:B3:51:LYS:HD3   | 2.25                     | 0.76              |
| 23:DB:458:G:C5'    | 49:D2:39:ARG:HB2   | 2.13                     | 0.76              |
| 23:DB:526:A:N6     | 23:DB:2626:C:H4'   | 2.00                     | 0.76              |
| 23:DB:1486:U:H2'   | 23:DB:1487:U:C6    | 2.21                     | 0.76              |
| 23:DB:2071:A:H2'   | 23:DB:2072:C:C6    | 2.20                     | 0.76              |
| 50:D3:48:MET:HE3   | 50:D3:49:VAL:H     | 1.50                     | 0.76              |
| 52:DI:25:PRO:O     | 52:DI:29:GLN:HG3   | 1.84                     | 0.76              |
| 15:AP:51:ARG:HB3   | 15:AP:51:ARG:HH11  | 1.48                     | 0.76              |
| 31:BJ:7:LYS:HD3    | 31:BJ:48:VAL:HB    | 1.67                     | 0.76              |
| 39:BR:47:VAL:HG22  | 39:BR:48:LYS:H     | 1.48                     | 0.76              |
| 11:CL:78:VAL:HG12  | 11:CL:101:LEU:HD13 | 1.67                     | 0.76              |
| 23:DB:1826:G:OP2   | 25:DC:221:GLY:HA2  | 1.86                     | 0.76              |
| 23:DB:2886:A:C8    | 47:D0:27:LEU:HG    | 2.21                     | 0.76              |
| 26:DD:8:LYS:HD3    | 37:DP:5:LYS:HE3    | 1.67                     | 0.76              |
| 1:AA:1057:G:H5''   | 2:AC:153:SER:HB3   | 1.67                     | 0.76              |
| 1:AA:1123:U:O2'    | 1:AA:1124:G:H5'    | 1.85                     | 0.76              |
| 20:AB:202:ASN:ND2  | 20:AB:204:ASP:H    | 1.83                     | 0.76              |
| 25:BC:106:PRO:HD2  | 25:BC:109:LEU:HD22 | 1.68                     | 0.76              |
| 30:BH:3:VAL:HG22   | 30:BH:21:VAL:HG11  | 1.67                     | 0.76              |
| 4:CE:110:MET:SD    | 4:CE:126:ALA:HB2   | 2.25                     | 0.76              |
| 8:CI:118:ARG:HH21  | 8:CI:122:ARG:NE    | 1.82                     | 0.76              |
| 9:CJ:57:VAL:HG22   | 9:CJ:58:ASN:H      | 1.49                     | 0.76              |
| 20:CB:132:GLU:HA   | 20:CB:135:MET:HE2  | 1.68                     | 0.76              |
| 23:DB:1113:U:H5''  | 29:DG:2:ARG:CZ     | 2.16                     | 0.76              |
| 24:DV:30:ILE:HG12  | 24:DV:91:PHE:HB2   | 1.65                     | 0.76              |
| 26:DD:5:VAL:HB     | 26:DD:27:ILE:O     | 1.85                     | 0.76              |
| 37:DP:76:HIS:H     | 37:DP:76:HIS:HD2   | 1.30                     | 0.76              |
| 10:AK:111:ASP:HB2  | 21:AU:16:ARG:HH22  | 1.50                     | 0.76              |
| 21:AU:17:ARG:HA    | 21:AU:20:ARG:HB3   | 1.66                     | 0.76              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:BC:224:MET:HA  | 25:BC:232:GLY:HA2  | 1.67                     | 0.76              |
| 36:BO:19:GLN:H    | 43:BW:76:ARG:HH12  | 1.32                     | 0.76              |
| 3:CD:138:PRO:HA   | 3:CD:181:PHE:HD2   | 1.50                     | 0.76              |
| 23:DB:2008:C:H2'  | 23:DB:2009:A:H8    | 1.51                     | 0.76              |
| 27:DE:14:VAL:HG12 | 27:DE:15:SER:H     | 1.48                     | 0.76              |
| 11:AL:78:VAL:HG12 | 11:AL:101:LEU:HD23 | 1.67                     | 0.76              |
| 11:AL:105:GLY:HA3 | 11:AL:117:GLY:HA3  | 1.67                     | 0.76              |
| 23:BB:811:U:C5    | 33:BL:29:LYS:HD3   | 2.20                     | 0.76              |
| 1:CA:1225:A:H5'   | 12:CM:101:THR:OG1  | 1.84                     | 0.76              |
| 4:CE:98:ALA:HB2   | 4:CE:123:LEU:HG    | 1.68                     | 0.76              |
| 38:DQ:30:VAL:HG12 | 38:DQ:31:TYR:N     | 2.00                     | 0.76              |
| 1:AA:1251:A:H2'   | 1:AA:1252:A:C8     | 2.21                     | 0.76              |
| 23:BB:27:G:H22    | 23:BB:512:G:H2'    | 1.50                     | 0.76              |
| 23:BB:1022:G:N7   | 31:BJ:68:LYS:HE3   | 2.01                     | 0.76              |
| 23:BB:1252:G:H1   | 38:BQ:36:GLN:NE2   | 1.83                     | 0.76              |
| 25:BC:77:VAL:HG23 | 25:BC:115:ILE:HD11 | 1.66                     | 0.76              |
| 47:B0:6:LYS:HA    | 47:B0:6:LYS:NZ     | 1.99                     | 0.76              |
| 1:CA:939:G:H5''   | 6:CG:101:ARG:HH12  | 1.49                     | 0.76              |
| 1:CA:1186:G:H21   | 13:CN:100:TRP:C    | 1.93                     | 0.76              |
| 23:DB:1368:G:C5'  | 49:D2:25:LYS:HG2   | 2.15                     | 0.76              |
| 34:DM:20:LEU:HD13 | 34:DM:38:ARG:HG3   | 1.67                     | 0.76              |
| 47:D0:41:HIS:CG   | 47:D0:42:ILE:H     | 2.03                     | 0.76              |
| 4:AE:131:ASN:HD21 | 4:AE:133:ILE:HB    | 1.50                     | 0.76              |
| 11:AL:87:LYS:HZ3  | 11:AL:87:LYS:HA    | 1.51                     | 0.76              |
| 23:BB:2420:C:OP1  | 50:B3:34:LYS:HB2   | 1.86                     | 0.76              |
| 23:BB:2443:C:H2'  | 23:BB:2444:G:H8    | 1.51                     | 0.76              |
| 25:BC:9:SER:HB2   | 25:BC:202:ARG:NE   | 2.00                     | 0.76              |
| 27:BE:4:VAL:HG22  | 27:BE:5:LEU:HD12   | 1.65                     | 0.76              |
| 40:BS:73:LYS:HB2  | 40:BS:106:VAL:HB   | 1.67                     | 0.76              |
| 48:B1:42:VAL:HG12 | 48:B1:43:ARG:HG3   | 1.67                     | 0.76              |
| 1:CA:814:A:H5'    | 1:CA:1511:G:H4'    | 1.66                     | 0.76              |
| 4:CE:47:PHE:HE1   | 4:CE:137:ARG:HE    | 1.34                     | 0.76              |
| 28:DF:132:ARG:HD3 | 28:DF:133:GLU:H    | 1.48                     | 0.76              |
| 31:DJ:135:GLN:NE2 | 31:DJ:138:GLN:H    | 1.83                     | 0.76              |
| 46:DZ:41:HIS:CG   | 46:DZ:42:PRO:HD2   | 2.21                     | 0.76              |
| 23:BB:125:A:H3'   | 23:BB:126:A:C5'    | 2.15                     | 0.76              |
| 23:BB:643:A:C2    | 48:B1:42:VAL:HG13  | 2.21                     | 0.76              |
| 23:BB:1241:A:H2'  | 23:BB:1242:U:H5'   | 1.67                     | 0.76              |
| 35:BN:119:SER:HB2 | 35:BN:121:LYS:HG2  | 1.67                     | 0.76              |
| 37:BP:51:ASN:HA   | 37:BP:61:ARG:H     | 1.51                     | 0.76              |
| 11:CL:49:ARG:HG2  | 11:CL:89:LEU:HD21  | 1.66                     | 0.76              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:547:A:H2'    | 23:DB:547:A:N3     | 1.99                     | 0.76              |
| 23:DB:2346:A:H3'   | 23:DB:2347:C:H5''  | 1.68                     | 0.76              |
| 24:DV:9:ARG:HH12   | 24:DV:12:GLN:HA    | 1.49                     | 0.76              |
| 26:DD:116:LYS:HG2  | 26:DD:123:LYS:HE2  | 1.67                     | 0.76              |
| 30:DH:94:ILE:HG22  | 30:DH:122:LEU:HG   | 1.68                     | 0.76              |
| 38:DQ:48:ASP:HA    | 38:DQ:51:GLN:NE2   | 2.00                     | 0.76              |
| 8:AI:71:ILE:H      | 8:AI:71:ILE:HD12   | 1.50                     | 0.76              |
| 28:BF:56:LEU:O     | 28:BF:59:ILE:HG22  | 1.86                     | 0.76              |
| 30:BH:73:ASN:N     | 30:BH:73:ASN:HD22  | 1.83                     | 0.76              |
| 52:BI:105:LEU:HD11 | 52:BI:139:VAL:HG11 | 1.66                     | 0.76              |
| 9:CJ:25:ILE:HG23   | 9:CJ:87:LEU:HD12   | 1.68                     | 0.76              |
| 23:DB:1098:A:P     | 52:DI:3:LYS:HG2    | 2.25                     | 0.76              |
| 23:DB:1175:A:H2'   | 23:DB:1176:U:H5'   | 1.68                     | 0.76              |
| 33:DL:19:LEU:H     | 33:DL:19:LEU:HD22  | 1.51                     | 0.76              |
| 8:AI:33:SER:HB3    | 8:AI:36:GLN:HB2    | 1.68                     | 0.76              |
| 10:AK:88:PRO:HD3   | 21:AU:28:LEU:HD13  | 1.68                     | 0.76              |
| 12:AM:44:ILE:HD12  | 12:AM:45:SER:H     | 1.51                     | 0.76              |
| 16:AQ:16:MET:HB2   | 16:AQ:19:SER:HB2   | 1.66                     | 0.76              |
| 20:AB:41:ASN:ND2   | 20:AB:44:LYS:HB2   | 2.00                     | 0.76              |
| 23:BB:118:A:H5'    | 23:BB:119:A:H8     | 1.49                     | 0.76              |
| 25:BC:127:ASN:HD22 | 25:BC:128:THR:H    | 1.31                     | 0.76              |
| 36:BO:76:LYS:HG2   | 36:BO:110:ALA:HB2  | 1.68                     | 0.76              |
| 44:BX:45:GLN:H     | 44:BX:45:GLN:NE2   | 1.83                     | 0.76              |
| 1:CA:1071:C:H2'    | 1:CA:1072:G:H8     | 1.52                     | 0.76              |
| 7:CH:72:GLU:H      | 7:CH:129:ALA:HB2   | 1.51                     | 0.76              |
| 23:DB:974:G:H1'    | 23:DB:975:A:C8     | 2.21                     | 0.76              |
| 26:DD:60:VAL:HG23  | 26:DD:63:PRO:HG2   | 1.66                     | 0.76              |
| 2:AC:8:GLY:HA2     | 2:AC:11:LEU:HG     | 1.69                     | 0.75              |
| 2:AC:146:LYS:HE3   | 2:AC:202:PHE:HE2   | 1.51                     | 0.75              |
| 2:AC:156:LEU:HD11  | 2:AC:163:ARG:O     | 1.87                     | 0.75              |
| 3:AD:137:SER:HB2   | 3:AD:138:PRO:HD2   | 1.68                     | 0.75              |
| 16:AQ:45:VAL:HG12  | 16:AQ:46:HIS:H     | 1.49                     | 0.75              |
| 23:BB:2301:C:H2'   | 23:BB:2302:U:C6    | 2.21                     | 0.75              |
| 25:BC:229:HIS:HE2  | 25:BC:244:VAL:HG22 | 1.48                     | 0.75              |
| 31:BJ:7:LYS:HD2    | 31:BJ:49:ASP:HB2   | 1.66                     | 0.75              |
| 33:BL:91:ASP:O     | 33:BL:92:LEU:HB2   | 1.86                     | 0.75              |
| 34:BM:42:THR:HG22  | 34:BM:45:GLN:HB2   | 1.67                     | 0.75              |
| 35:BN:38:LEU:HB2   | 35:BN:109:PRO:HB2  | 1.68                     | 0.75              |
| 42:BU:78:LYS:HE3   | 42:BU:96:LYS:HB2   | 1.66                     | 0.75              |
| 50:B3:12:ARG:HB2   | 50:B3:12:ARG:HH11  | 1.48                     | 0.75              |
| 22:DA:47:C:OP1     | 36:DO:1:MET:HA     | 1.87                     | 0.75              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:DV:63:ILE:N    | 24:DV:70:ILE:HD11  | 1.99                     | 0.75              |
| 49:D2:43:THR:O    | 49:D2:44:VAL:HG13  | 1.85                     | 0.75              |
| 2:AC:49:ALA:HB1   | 2:AC:75:VAL:HG22   | 1.68                     | 0.75              |
| 5:AF:92:THR:HG23  | 5:AF:93:LYS:H      | 1.51                     | 0.75              |
| 23:BB:78:U:H2'    | 23:BB:79:C:C6      | 2.21                     | 0.75              |
| 23:BB:633:A:H8    | 23:BB:633:A:O5'    | 1.70                     | 0.75              |
| 27:BE:141:MET:HG3 | 27:BE:143:LEU:H    | 1.52                     | 0.75              |
| 33:BL:94:THR:HB   | 33:BL:103:ILE:HG12 | 1.68                     | 0.75              |
| 20:CB:94:ARG:HE   | 20:CB:94:ARG:N     | 1.84                     | 0.75              |
| 20:CB:218:ALA:HA  | 20:CB:221:ARG:HG2  | 1.68                     | 0.75              |
| 23:DB:957:C:OP1   | 34:DM:76:LYS:HD3   | 1.86                     | 0.75              |
| 30:DH:75:LEU:HD23 | 30:DH:75:LEU:H     | 1.51                     | 0.75              |
| 49:D2:35:ARG:HH21 | 49:D2:42:LEU:HD12  | 1.51                     | 0.75              |
| 1:AA:967:C:H3'    | 1:AA:968:A:C5'     | 2.15                     | 0.75              |
| 3:AD:159:GLU:HG3  | 3:AD:160:LEU:H     | 1.50                     | 0.75              |
| 23:BB:855:G:H21   | 43:BW:23:LYS:HD2   | 1.50                     | 0.75              |
| 23:BB:1654:A:OP1  | 35:BN:1:MET:HB2    | 1.86                     | 0.75              |
| 34:BM:71:LYS:O    | 34:BM:71:LYS:HD2   | 1.86                     | 0.75              |
| 43:BW:23:LYS:HB2  | 43:BW:23:LYS:HZ2   | 1.51                     | 0.75              |
| 19:CT:53:MET:HE3  | 19:CT:54:GLN:HA    | 1.69                     | 0.75              |
| 23:DB:534:U:H5'   | 38:DQ:41:ALA:HA    | 1.66                     | 0.75              |
| 23:DB:1299:G:H4'  | 23:DB:1301:A:H1'   | 1.69                     | 0.75              |
| 23:DB:2012:G:OP1  | 40:DS:98:LYS:HD3   | 1.85                     | 0.75              |
| 23:DB:2204:G:O5'  | 25:DC:149:LYS:HE3  | 1.87                     | 0.75              |
| 26:DD:179:ARG:HB2 | 26:DD:188:LEU:HD22 | 1.68                     | 0.75              |
| 31:DJ:64:VAL:HG21 | 31:DJ:90:GLU:OE1   | 1.86                     | 0.75              |
| 35:DN:42:LYS:HE3  | 35:DN:45:ARG:HG3   | 1.67                     | 0.75              |
| 41:DT:14:PRO:HA   | 41:DT:32:LEU:HA    | 1.67                     | 0.75              |
| 41:DT:55:VAL:HG23 | 41:DT:87:LEU:N     | 2.01                     | 0.75              |
| 23:BB:2346:A:H3'  | 23:BB:2347:C:H5''  | 1.67                     | 0.75              |
| 26:BD:8:LYS:HB3   | 37:BP:5:LYS:NZ     | 2.01                     | 0.75              |
| 28:BF:102:LEU:O   | 28:BF:107:VAL:HG23 | 1.86                     | 0.75              |
| 29:BG:51:PHE:HE2  | 29:BG:63:GLN:HE21  | 1.34                     | 0.75              |
| 38:BQ:91:ARG:N    | 39:BR:10:LYS:HZ2   | 1.79                     | 0.75              |
| 45:BY:10:ARG:NE   | 45:BY:31:ILE:HG13  | 2.01                     | 0.75              |
| 47:B0:8:THR:HG23  | 47:B0:9:ARG:H      | 1.51                     | 0.75              |
| 1:CA:780:A:O2'    | 1:CA:781:A:H5''    | 1.87                     | 0.75              |
| 1:CA:1056:U:H5'   | 2:CC:162:ALA:HB2   | 1.65                     | 0.75              |
| 1:CA:1399:C:H4'   | 1:CA:1400:C:H5''   | 1.67                     | 0.75              |
| 1:CA:1508:A:H2'   | 1:CA:1509:C:C6     | 2.22                     | 0.75              |
| 7:CH:10:LEU:HD22  | 7:CH:74:ILE:HD11   | 1.68                     | 0.75              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:2443:C:H2'  | 23:DB:2444:G:H8    | 1.51                     | 0.75              |
| 26:DD:37:VAL:HB   | 26:DD:46:ARG:HB2   | 1.68                     | 0.75              |
| 42:DU:4:ILE:HG21  | 42:DU:27:VAL:HG13  | 1.68                     | 0.75              |
| 1:AA:575:G:H4'    | 1:AA:576:C:O5'     | 1.84                     | 0.75              |
| 1:AA:1409:C:H42   | 1:AA:1491:G:H1     | 1.33                     | 0.75              |
| 4:AE:95:MET:HE1   | 4:AE:114:LEU:HD21  | 1.66                     | 0.75              |
| 7:AH:30:LYS:HA    | 7:AH:30:LYS:NZ     | 2.01                     | 0.75              |
| 18:AS:4:LEU:C     | 18:AS:5:LYS:HE3    | 2.12                     | 0.75              |
| 23:BB:1197:G:H2'  | 23:BB:1198:U:H6    | 1.49                     | 0.75              |
| 23:BB:1440:U:H2'  | 23:BB:1441:G:H8    | 1.51                     | 0.75              |
| 23:BB:1486:U:H2'  | 23:BB:1487:U:C6    | 2.21                     | 0.75              |
| 26:BD:1:MET:HB2   | 26:BD:84:LEU:HD22  | 1.68                     | 0.75              |
| 27:BE:89:PRO:O    | 27:BE:90:GLN:HG2   | 1.85                     | 0.75              |
| 39:BR:58:VAL:HG22 | 39:BR:59:ILE:H     | 1.52                     | 0.75              |
| 44:BX:22:LEU:HD22 | 44:BX:26:PHE:HB2   | 1.69                     | 0.75              |
| 48:B1:12:SER:HB2  | 48:B1:21:THR:O     | 1.85                     | 0.75              |
| 52:BI:20:SER:HB3  | 52:BI:21:PRO:HD3   | 1.68                     | 0.75              |
| 1:CA:817:C:H1'    | 1:CA:819:A:H5'     | 1.69                     | 0.75              |
| 3:CD:2:ARG:NH1    | 3:CD:114:ARG:HD3   | 2.00                     | 0.75              |
| 23:DB:898:C:O2'   | 23:DB:899:A:H5''   | 1.86                     | 0.75              |
| 24:DV:72:VAL:HG12 | 24:DV:93:ARG:HA    | 1.68                     | 0.75              |
| 42:DU:3:LYS:HD3   | 42:DU:81:ARG:HH12  | 1.52                     | 0.75              |
| 1:AA:814:A:H5'    | 1:AA:1511:G:H4'    | 1.69                     | 0.75              |
| 2:AC:153:SER:HB2  | 2:AC:196:GLY:H     | 1.51                     | 0.75              |
| 19:AT:59:ARG:HH11 | 19:AT:59:ARG:HB2   | 1.51                     | 0.75              |
| 23:BB:65:U:OP1    | 41:BT:76:ARG:HB2   | 1.87                     | 0.75              |
| 26:BD:91:THR:HG23 | 26:BD:92:VAL:H     | 1.50                     | 0.75              |
| 27:BE:120:VAL:H   | 27:BE:189:THR:HG22 | 1.50                     | 0.75              |
| 28:BF:35:LEU:HA   | 28:BF:153:ILE:HA   | 1.67                     | 0.75              |
| 1:CA:269:C:H2'    | 1:CA:270:A:H8      | 1.50                     | 0.75              |
| 4:CE:44:ARG:HA    | 4:CE:71:ILE:O      | 1.85                     | 0.75              |
| 23:DB:544:C:H2'   | 23:DB:545:U:C4     | 2.21                     | 0.75              |
| 23:DB:1825:U:H5'  | 25:DC:244:VAL:CG2  | 2.16                     | 0.75              |
| 30:DH:11:ASN:HD22 | 30:DH:20:ASN:HD22  | 1.33                     | 0.75              |
| 1:AA:780:A:O2'    | 1:AA:781:A:H5''    | 1.87                     | 0.75              |
| 16:AQ:18:LYS:HG2  | 16:AQ:48:GLU:HA    | 1.68                     | 0.75              |
| 31:BJ:45:THR:HB   | 38:BQ:63:ARG:NH2   | 2.01                     | 0.75              |
| 1:CA:1412:C:H2'   | 1:CA:1413:A:C8     | 2.21                     | 0.75              |
| 2:CC:182:ASP:HB2  | 2:CC:203:LYS:HE2   | 1.67                     | 0.75              |
| 23:DB:90:U:H3'    | 23:DB:91:A:C5'     | 2.17                     | 0.75              |
| 23:DB:718:A:H2'   | 23:DB:719:C:H5'    | 1.67                     | 0.75              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:2756:U:H1'  | 23:DB:2757:A:H5''  | 1.69                     | 0.75              |
| 26:DD:24:VAL:HG11 | 26:DD:193:VAL:HG11 | 1.69                     | 0.75              |
| 31:DJ:133:ALA:HA  | 31:DJ:136:GLN:HB2  | 1.66                     | 0.75              |
| 37:DP:28:LYS:H    | 37:DP:86:LYS:HD3   | 1.52                     | 0.75              |
| 1:AA:65:A:H2'     | 1:AA:65:A:N3       | 2.00                     | 0.75              |
| 1:AA:1111:A:HO2'  | 1:AA:1112:C:H6     | 1.30                     | 0.75              |
| 11:AL:20:VAL:HG13 | 11:AL:94:TYR:HH    | 1.49                     | 0.75              |
| 25:BC:235:GLU:HG3 | 25:BC:237:ARG:HD3  | 1.67                     | 0.75              |
| 42:BU:7:ASP:N     | 42:BU:24:VAL:HA    | 2.01                     | 0.75              |
| 23:DB:704:G:O2'   | 23:DB:727:A:N6     | 2.19                     | 0.75              |
| 23:DB:2204:G:H4'  | 25:DC:149:LYS:HG3  | 1.69                     | 0.75              |
| 31:DJ:40:HIS:HA   | 38:DQ:69:ARG:HH12  | 1.50                     | 0.75              |
| 36:DO:72:ALA:O    | 36:DO:76:LYS:HE3   | 1.87                     | 0.75              |
| 1:AA:269:C:H2'    | 1:AA:270:A:H8      | 1.50                     | 0.75              |
| 1:AA:1326:U:H2'   | 1:AA:1327:C:C6     | 2.21                     | 0.75              |
| 6:AG:67:ASN:HD22  | 6:AG:127:ALA:HA    | 1.51                     | 0.75              |
| 23:BB:742:A:H2'   | 23:BB:743:A:C8     | 2.21                     | 0.75              |
| 26:BD:154:LYS:C   | 26:BD:156:PHE:H    | 1.94                     | 0.75              |
| 29:BG:157:LYS:HG3 | 29:BG:159:LYS:HZ2  | 1.51                     | 0.75              |
| 34:BM:42:THR:HA   | 34:BM:92:TRP:HD1   | 1.51                     | 0.75              |
| 52:BI:122:GLU:O   | 52:BI:126:ARG:HG3  | 1.87                     | 0.75              |
| 4:CE:95:MET:HE3   | 4:CE:143:LEU:HD13  | 1.68                     | 0.75              |
| 23:DB:1060:U:C5   | 52:DI:131:THR:HG22 | 2.22                     | 0.75              |
| 25:DC:257:ARG:HA  | 25:DC:261:ARG:HD2  | 1.68                     | 0.75              |
| 32:DK:102:PRO:HB3 | 32:DK:121:GLU:HG2  | 1.69                     | 0.75              |
| 33:DL:55:MET:HB3  | 33:DL:56:PRO:HD3   | 1.69                     | 0.75              |
| 37:DP:47:ILE:HG22 | 37:DP:48:ALA:N     | 2.00                     | 0.75              |
| 1:AA:1125:U:H2'   | 1:AA:1126:U:H5''   | 1.68                     | 0.74              |
| 16:AQ:10:ARG:NH1  | 16:AQ:56:ASP:H     | 1.85                     | 0.74              |
| 23:BB:508:A:H2'   | 23:BB:509:C:H5'    | 1.66                     | 0.74              |
| 23:BB:590:A:H2'   | 23:BB:591:U:C6     | 2.22                     | 0.74              |
| 25:BC:77:VAL:HG21 | 25:BC:109:LEU:HG   | 1.69                     | 0.74              |
| 33:BL:78:ARG:HG2  | 33:BL:99:ASN:HB3   | 1.69                     | 0.74              |
| 1:CA:1277:C:O2'   | 1:CA:1279:G:H1'    | 1.86                     | 0.74              |
| 8:CI:27:ILE:HD13  | 8:CI:34:LEU:HD13   | 1.68                     | 0.74              |
| 23:DB:590:A:H2'   | 23:DB:591:U:C6     | 2.22                     | 0.74              |
| 23:DB:1099:G:C8   | 52:DI:3:LYS:HB2    | 2.22                     | 0.74              |
| 23:DB:2751:G:H5'  | 29:DG:3:VAL:CG2    | 2.16                     | 0.74              |
| 27:DE:142:ALA:N   | 27:DE:185:LYS:HZ1  | 1.83                     | 0.74              |
| 35:DN:8:ARG:HD2   | 35:DN:46:ARG:HE    | 1.48                     | 0.74              |
| 1:AA:1000:A:H2'   | 1:AA:1001:C:C6     | 2.22                     | 0.74              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:AL:35:ARG:HA    | 11:AL:35:ARG:HE    | 1.52                     | 0.74              |
| 20:AB:61:SER:HA    | 20:AB:224:ARG:HA   | 1.69                     | 0.74              |
| 23:BB:394:C:H2'    | 23:BB:395:U:O4'    | 1.86                     | 0.74              |
| 23:BB:1178:C:H2'   | 23:BB:1179:G:H8    | 1.51                     | 0.74              |
| 23:BB:2471:A:O2'   | 23:BB:2472:G:H8    | 1.70                     | 0.74              |
| 23:BB:2840:C:H5''  | 35:BN:53:THR:HG21  | 1.69                     | 0.74              |
| 25:BC:110:LYS:HE3  | 25:BC:111:ALA:H    | 1.52                     | 0.74              |
| 27:BE:52:VAL:HG22  | 27:BE:53:THR:H     | 1.52                     | 0.74              |
| 41:BT:29:THR:HG22  | 41:BT:86:THR:HG22  | 1.69                     | 0.74              |
| 1:CA:1316:G:H2'    | 1:CA:1318:A:OP2    | 1.87                     | 0.74              |
| 3:CD:57:LYS:HB2    | 3:CD:199:ILE:HB    | 1.68                     | 0.74              |
| 15:CP:4:ILE:HG12   | 15:CP:21:VAL:HG22  | 1.67                     | 0.74              |
| 20:CB:18:GLN:O     | 20:CB:37:VAL:HG23  | 1.86                     | 0.74              |
| 23:DB:742:A:H2'    | 23:DB:743:A:C8     | 2.21                     | 0.74              |
| 25:DC:15:VAL:HG13  | 25:DC:16:VAL:HG23  | 1.67                     | 0.74              |
| 25:DC:193:GLU:O    | 25:DC:194:VAL:HG13 | 1.87                     | 0.74              |
| 37:DP:32:VAL:HB    | 37:DP:80:VAL:HG13  | 1.69                     | 0.74              |
| 49:D2:25:LYS:N     | 49:D2:25:LYS:HD2   | 2.01                     | 0.74              |
| 23:BB:107:G:H21    | 23:BB:346:A:N6     | 1.84                     | 0.74              |
| 23:BB:275:C:H2'    | 23:BB:276:U:O4'    | 1.86                     | 0.74              |
| 23:BB:1009:A:O2'   | 38:BQ:61:ILE:HD11  | 1.86                     | 0.74              |
| 23:BB:1113:U:H5''  | 29:BG:1:SER:HA     | 1.69                     | 0.74              |
| 23:BB:1727:C:H2'   | 23:BB:1728:C:C6    | 2.22                     | 0.74              |
| 23:BB:2086:U:H2'   | 23:BB:2087:G:C8    | 2.22                     | 0.74              |
| 26:BD:35:THR:HG22  | 26:BD:46:ARG:HH22  | 1.52                     | 0.74              |
| 46:BZ:53:THR:HA    | 46:BZ:56:ARG:HD2   | 1.68                     | 0.74              |
| 1:CA:878:A:O4'     | 7:CH:3:GLN:HG3     | 1.88                     | 0.74              |
| 3:CD:117:VAL:HG12  | 3:CD:130:ASN:HA    | 1.70                     | 0.74              |
| 20:CB:81:ASP:HA    | 20:CB:84:LEU:HD22  | 1.68                     | 0.74              |
| 39:DR:4:VAL:HG12   | 39:DR:43:ASN:HB3   | 1.69                     | 0.74              |
| 47:D0:32:THR:HG21  | 47:D0:41:HIS:NE2   | 2.01                     | 0.74              |
| 49:D2:35:ARG:NH2   | 49:D2:43:THR:H     | 1.86                     | 0.74              |
| 1:AA:1446:A:H2'    | 1:AA:1447:A:H5''   | 1.69                     | 0.74              |
| 21:AU:40:PRO:HG2   | 21:AU:41:THR:H     | 1.51                     | 0.74              |
| 23:BB:643:A:H2     | 48:B1:42:VAL:HG13  | 1.52                     | 0.74              |
| 23:BB:857:G:O2'    | 23:BB:858:G:H5'    | 1.86                     | 0.74              |
| 33:BL:118:THR:CG2  | 33:BL:119:PRO:HD3  | 2.17                     | 0.74              |
| 1:CA:270:A:H2'     | 1:CA:271:C:C6      | 2.23                     | 0.74              |
| 1:CA:1436:U:H2'    | 1:CA:1437:A:H8     | 1.52                     | 0.74              |
| 2:CC:95:GLY:O      | 2:CC:96:VAL:HG13   | 1.86                     | 0.74              |
| 10:CK:110:THR:HG22 | 21:CU:5:VAL:H      | 1.52                     | 0.74              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:DH:6:LEU:HD12   | 30:DH:36:ALA:N     | 2.02                     | 0.74              |
| 36:DO:100:HIS:O    | 36:DO:104:GLN:HB3  | 1.87                     | 0.74              |
| 38:DQ:7:VAL:HG13   | 38:DQ:8:ILE:HD12   | 1.67                     | 0.74              |
| 11:AL:22:ALA:HB1   | 11:AL:29:LYS:HG3   | 1.70                     | 0.74              |
| 12:AM:78:ARG:NH2   | 12:AM:79:LEU:HG    | 2.03                     | 0.74              |
| 25:BC:146:LYS:HB3  | 25:BC:147:PRO:HD2  | 1.69                     | 0.74              |
| 25:BC:222:THR:HA   | 25:BC:231:HIS:NE2  | 2.02                     | 0.74              |
| 30:BH:26:ALA:HB1   | 30:BH:31:VAL:HG23  | 1.70                     | 0.74              |
| 34:BM:8:LYS:HZ2    | 34:BM:70:ASP:H     | 1.34                     | 0.74              |
| 35:BN:62:ASN:ND2   | 35:BN:80:PHE:HB3   | 2.02                     | 0.74              |
| 35:BN:82:GLU:O     | 35:BN:86:ARG:HG3   | 1.88                     | 0.74              |
| 38:BQ:47:ARG:HH22  | 38:BQ:50:ARG:HB3   | 1.51                     | 0.74              |
| 38:BQ:106:THR:O    | 38:BQ:109:VAL:HG22 | 1.86                     | 0.74              |
| 41:BT:5:GLU:HG2    | 41:BT:6:ARG:N      | 2.02                     | 0.74              |
| 1:CA:430:A:OP1     | 3:CD:8:LEU:HB2     | 1.86                     | 0.74              |
| 1:CA:1219:A:H5'    | 13:CN:52:ARG:HH12  | 1.52                     | 0.74              |
| 14:CO:21:THR:HA    | 14:CO:26:VAL:HG11  | 1.69                     | 0.74              |
| 16:CQ:5:ARG:HB3    | 16:CQ:7:LEU:HD23   | 1.70                     | 0.74              |
| 42:DU:46:LYS:HE2   | 42:DU:53:GLN:HA    | 1.69                     | 0.74              |
| 1:AA:1008:U:H2'    | 1:AA:1009:U:H4'    | 1.68                     | 0.74              |
| 2:AC:179:ALA:HB1   | 2:AC:202:PHE:HE1   | 1.50                     | 0.74              |
| 4:AE:87:VAL:HG12   | 4:AE:92:ARG:HA     | 1.68                     | 0.74              |
| 40:BS:89:ALA:C     | 40:BS:90:LYS:HZ3   | 1.94                     | 0.74              |
| 45:BY:54:VAL:HG22  | 45:BY:55:LYS:H     | 1.52                     | 0.74              |
| 23:DB:2102:G:H2'   | 23:DB:2103:C:O4'   | 1.87                     | 0.74              |
| 23:DB:2144:G:O2'   | 23:DB:2145:C:H5'   | 1.87                     | 0.74              |
| 30:DH:121:VAL:HG23 | 30:DH:122:LEU:HD23 | 1.68                     | 0.74              |
| 40:DS:6:LYS:HA     | 40:DS:104:THR:HA   | 1.68                     | 0.74              |
| 43:DW:42:THR:HG23  | 43:DW:66:VAL:H     | 1.53                     | 0.74              |
| 23:BB:19:A:H2'     | 23:BB:20:C:C6      | 2.23                     | 0.74              |
| 23:BB:1437:C:H2'   | 23:BB:1438:U:C6    | 2.22                     | 0.74              |
| 27:BE:47:LYS:H     | 27:BE:47:LYS:CD    | 1.98                     | 0.74              |
| 30:BH:89:LYS:HZ1   | 30:BH:123:ARG:HB3  | 1.53                     | 0.74              |
| 33:BL:77:ILE:HG22  | 33:BL:78:ARG:HG3   | 1.69                     | 0.74              |
| 44:BX:22:LEU:HD22  | 44:BX:26:PHE:H     | 1.52                     | 0.74              |
| 49:B2:22:MET:HE2   | 49:B2:31:LEU:HG    | 1.69                     | 0.74              |
| 1:CA:1170:A:H2'    | 1:CA:1171:A:O4'    | 1.88                     | 0.74              |
| 43:DW:3:LYS:HA     | 43:DW:3:LYS:HZ3    | 1.50                     | 0.74              |
| 49:D2:25:LYS:HD2   | 49:D2:25:LYS:H     | 1.52                     | 0.74              |
| 13:AN:42:ASN:HB3   | 13:AN:46:LYS:HE2   | 1.70                     | 0.74              |
| 20:AB:120:SER:HA   | 20:AB:125:PHE:HB3  | 1.68                     | 0.74              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:BA:60:C:H2'     | 22:BA:61:G:H8     | 1.53                     | 0.74              |
| 23:BB:2420:C:OP1   | 50:B3:34:LYS:HE3  | 1.87                     | 0.74              |
| 32:BK:11:ALA:HB3   | 32:BK:85:VAL:CG2  | 2.17                     | 0.74              |
| 33:BL:110:VAL:HB   | 33:BL:126:ARG:NH2 | 2.02                     | 0.74              |
| 34:BM:95:LEU:HD22  | 34:BM:98:PRO:HG3  | 1.69                     | 0.74              |
| 42:BU:81:ARG:HA    | 42:BU:81:ARG:HH11 | 1.52                     | 0.74              |
| 43:BW:48:ALA:HB3   | 43:BW:72:GLY:HA3  | 1.68                     | 0.74              |
| 18:CS:50:VAL:HG21  | 18:CS:70:LEU:HG   | 1.70                     | 0.74              |
| 23:DB:704:G:H1'    | 23:DB:727:A:N6    | 2.03                     | 0.74              |
| 23:DB:1063:G:H1'   | 52:DI:92:PRO:HG2  | 1.70                     | 0.74              |
| 23:DB:2257:U:H5'   | 43:DW:5:ALA:HB2   | 1.69                     | 0.74              |
| 1:AA:1294:G:H2'    | 1:AA:1295:U:C6    | 2.22                     | 0.74              |
| 9:AJ:92:LEU:H      | 9:AJ:92:LEU:HD22  | 1.52                     | 0.74              |
| 23:BB:37:C:C2'     | 27:BE:46:GLN:HG2  | 2.17                     | 0.74              |
| 23:BB:192:C:H2'    | 23:BB:193:U:H5'   | 1.69                     | 0.74              |
| 26:BD:13:ARG:HA    | 26:BD:13:ARG:HH11 | 1.53                     | 0.74              |
| 26:BD:107:VAL:HA   | 26:BD:205:PRO:O   | 1.87                     | 0.74              |
| 26:BD:110:THR:HG22 | 26:BD:171:THR:HA  | 1.70                     | 0.74              |
| 48:B1:53:ILE:HD13  | 48:B1:54:LYS:N    | 2.03                     | 0.74              |
| 49:B2:13:ASN:HA    | 49:B2:18:PHE:HB2  | 1.69                     | 0.74              |
| 4:CE:82:HIS:HB2    | 4:CE:83:PRO:HD2   | 1.70                     | 0.74              |
| 8:CI:4:GLN:HG2     | 8:CI:21:LYS:HD3   | 1.69                     | 0.74              |
| 22:DA:17:C:H2'     | 22:DA:18:G:O4'    | 1.88                     | 0.74              |
| 23:DB:633:A:H8     | 23:DB:633:A:O5'   | 1.69                     | 0.74              |
| 23:DB:1081:U:H5'   | 52:DI:126:ARG:NH1 | 2.02                     | 0.74              |
| 23:DB:1785:A:H2'   | 23:DB:1787:A:N7   | 2.03                     | 0.74              |
| 29:DG:155:PRO:HB3  | 29:DG:171:LYS:HB3 | 1.68                     | 0.74              |
| 36:DO:21:LEU:HD23  | 36:DO:22:GLY:H    | 1.51                     | 0.74              |
| 52:DI:20:SER:HB3   | 52:DI:21:PRO:HD3  | 1.68                     | 0.74              |
| 1:AA:270:A:H2'     | 1:AA:271:C:C6     | 2.23                     | 0.74              |
| 1:AA:817:C:H1'     | 1:AA:819:A:H5'    | 1.69                     | 0.74              |
| 4:AE:108:GLY:H     | 4:AE:110:MET:HE1  | 1.53                     | 0.74              |
| 13:AN:30:ILE:HG21  | 13:AN:41:TRP:HB2  | 1.68                     | 0.74              |
| 15:AP:42:ILE:HG22  | 15:AP:43:ALA:H    | 1.52                     | 0.74              |
| 23:BB:467:G:OP1    | 49:B2:33:ARG:HD3  | 1.88                     | 0.74              |
| 23:BB:588:U:OP1    | 33:BL:27:LEU:HB2  | 1.86                     | 0.74              |
| 23:BB:1176:U:H2'   | 23:BB:1177:G:O4'  | 1.88                     | 0.74              |
| 23:BB:1252:G:O6    | 38:BQ:35:PHE:HB2  | 1.88                     | 0.74              |
| 52:BI:7:TYR:HB2    | 52:BI:58:ILE:O    | 1.88                     | 0.74              |
| 23:DB:704:G:H1'    | 23:DB:727:A:H61   | 1.52                     | 0.74              |
| 23:DB:1727:C:H2'   | 23:DB:1728:C:C6   | 2.22                     | 0.74              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:DD:33:ARG:HB2   | 26:DD:33:ARG:HH11  | 1.51                     | 0.74              |
| 1:AA:501:C:H2'     | 1:AA:502:A:H8      | 1.52                     | 0.73              |
| 20:AB:150:ILE:HG13 | 20:AB:153:MET:HE3  | 1.70                     | 0.73              |
| 23:BB:2301:C:H2'   | 23:BB:2302:U:H6    | 1.52                     | 0.73              |
| 37:BP:62:LYS:HE3   | 37:BP:74:GLN:HE22  | 1.53                     | 0.73              |
| 1:CA:239:U:H4'     | 1:CA:239:U:OP1     | 1.88                     | 0.73              |
| 1:CA:501:C:H2'     | 1:CA:502:A:H8      | 1.52                     | 0.73              |
| 1:CA:812:G:H2'     | 1:CA:812:G:N3      | 2.02                     | 0.73              |
| 23:DB:143:C:O2     | 41:DT:3:ARG:HD2    | 1.88                     | 0.73              |
| 23:DB:643:A:N6     | 23:DB:2370:G:H1'   | 2.01                     | 0.73              |
| 24:DV:63:ILE:H     | 24:DV:70:ILE:CD1   | 1.99                     | 0.73              |
| 27:DE:6:LYS:HG2    | 27:DE:119:ILE:HB   | 1.69                     | 0.73              |
| 2:AC:185:THR:HG22  | 2:AC:186:SER:H     | 1.52                     | 0.73              |
| 23:BB:1534:U:HO2'  | 23:BB:1535:A:H8    | 1.35                     | 0.73              |
| 23:BB:2239:G:H5'   | 25:BC:246:PRO:CD   | 2.19                     | 0.73              |
| 23:BB:2511:U:H4'   | 26:BD:128:ARG:NH2  | 2.03                     | 0.73              |
| 25:BC:107:LYS:CB   | 25:BC:194:VAL:HG11 | 2.17                     | 0.73              |
| 30:BH:84:ALA:HA    | 30:BH:90:LEU:HG    | 1.70                     | 0.73              |
| 33:BL:110:VAL:H    | 33:BL:126:ARG:HB2  | 1.52                     | 0.73              |
| 34:BM:114:ARG:HH21 | 34:BM:125:PRO:HA   | 1.53                     | 0.73              |
| 40:BS:34:ASP:N     | 40:BS:37:THR:HG22  | 2.03                     | 0.73              |
| 42:BU:90:LYS:HZ2   | 42:BU:91:LYS:HE2   | 1.52                     | 0.73              |
| 51:B4:25:VAL:HG23  | 51:B4:35:GLN:HB2   | 1.68                     | 0.73              |
| 1:CA:619:U:H3      | 3:CD:130:ASN:ND2   | 1.87                     | 0.73              |
| 6:CG:58:LEU:H      | 6:CG:58:LEU:HD23   | 1.51                     | 0.73              |
| 8:CI:114:LYS:HB2   | 8:CI:117:LEU:HD12  | 1.70                     | 0.73              |
| 23:DB:1437:C:H2'   | 23:DB:1438:U:C6    | 2.22                     | 0.73              |
| 26:DD:189:VAL:HG12 | 26:DD:190:LYS:H    | 1.52                     | 0.73              |
| 52:DI:121:ILE:HD13 | 52:DI:121:ILE:H    | 1.52                     | 0.73              |
| 23:BB:1299:G:H4'   | 23:BB:1301:A:H1'   | 1.68                     | 0.73              |
| 23:BB:1392:A:N6    | 41:BT:18:GLU:HG2   | 2.04                     | 0.73              |
| 23:BB:1785:A:H2'   | 23:BB:1787:A:N7    | 2.03                     | 0.73              |
| 23:BB:2575:C:H4'   | 26:BD:148:GLN:CA   | 2.17                     | 0.73              |
| 26:BD:138:LEU:HD23 | 26:BD:138:LEU:H    | 1.52                     | 0.73              |
| 45:BY:15:ARG:HE    | 45:BY:15:ARG:N     | 1.87                     | 0.73              |
| 45:BY:20:LYS:HA    | 45:BY:24:LEU:HB2   | 1.69                     | 0.73              |
| 48:B1:45:HIS:O     | 48:B1:46:VAL:HG12  | 1.87                     | 0.73              |
| 23:DB:578:G:N2     | 38:DQ:32:ARG:HH21  | 1.86                     | 0.73              |
| 26:DD:27:ILE:HD13  | 26:DD:28:GLU:N     | 2.03                     | 0.73              |
| 34:DM:2:LEU:H      | 34:DM:2:LEU:HD12   | 1.53                     | 0.73              |
| 35:DN:86:ARG:HB3   | 35:DN:86:ARG:NH1   | 2.02                     | 0.73              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:DP:6:GLN:CD     | 37:DP:6:GLN:H      | 1.95                     | 0.73              |
| 2:AC:155:ARG:H     | 2:AC:162:ALA:HA    | 1.52                     | 0.73              |
| 10:AK:113:THR:HG21 | 21:AU:28:LEU:HD11  | 1.71                     | 0.73              |
| 22:BA:50:A:H5''    | 36:BO:68:LYS:HD2   | 1.71                     | 0.73              |
| 25:BC:129:LEU:HD23 | 25:BC:130:PRO:HD2  | 1.70                     | 0.73              |
| 33:BL:95:LEU:HD12  | 33:BL:95:LEU:H     | 1.53                     | 0.73              |
| 38:BQ:65:ASN:HB2   | 38:BQ:75:TYR:HB2   | 1.69                     | 0.73              |
| 41:BT:30:ILE:HG23  | 41:BT:31:VAL:N     | 2.03                     | 0.73              |
| 43:BW:23:LYS:HB2   | 43:BW:23:LYS:NZ    | 2.04                     | 0.73              |
| 1:CA:268:U:H2'     | 1:CA:269:C:C6      | 2.23                     | 0.73              |
| 1:CA:1241:G:H2'    | 1:CA:1242:G:H8     | 1.52                     | 0.73              |
| 29:DG:5:LYS:HD3    | 29:DG:68:ARG:HB3   | 1.68                     | 0.73              |
| 43:DW:35:ILE:HG21  | 43:DW:70:VAL:HG11  | 1.71                     | 0.73              |
| 23:BB:1171:G:H2'   | 23:BB:1172:C:O4'   | 1.88                     | 0.73              |
| 23:BB:1714:U:H3'   | 23:BB:1715:G:C5'   | 2.18                     | 0.73              |
| 24:BV:70:ILE:HG12  | 24:BV:71:LYS:H     | 1.51                     | 0.73              |
| 25:BC:131:MET:HE1  | 25:BC:143:VAL:HG11 | 1.71                     | 0.73              |
| 26:BD:119:ALA:HA   | 26:BD:123:LYS:HZ1  | 1.54                     | 0.73              |
| 29:BG:26:LYS:HA    | 29:BG:31:GLU:HG2   | 1.70                     | 0.73              |
| 36:BO:50:ALA:HB2   | 36:BO:83:LEU:HD11  | 1.70                     | 0.73              |
| 1:CA:922:G:H2'     | 1:CA:923:A:C8      | 2.23                     | 0.73              |
| 23:DB:1820:U:H3    | 25:DC:197:ALA:HB1  | 1.53                     | 0.73              |
| 23:DB:2185:U:H2'   | 23:DB:2186:G:O4'   | 1.88                     | 0.73              |
| 23:DB:2895:G:H2'   | 23:DB:2896:C:C6    | 2.24                     | 0.73              |
| 34:DM:41:LEU:HD23  | 34:DM:67:VAL:HG21  | 1.71                     | 0.73              |
| 1:AA:268:U:H2'     | 1:AA:269:C:C6      | 2.23                     | 0.73              |
| 23:BB:2682:A:C2    | 26:BD:22:ILE:HD11  | 2.22                     | 0.73              |
| 28:BF:135:ILE:HD13 | 28:BF:138:PRO:HA   | 1.69                     | 0.73              |
| 35:BN:99:LYS:NZ    | 35:BN:99:LYS:HB3   | 2.03                     | 0.73              |
| 39:BR:41:ILE:C     | 39:BR:43:ASN:H     | 1.95                     | 0.73              |
| 13:CN:9:GLU:HA     | 13:CN:12:ARG:HB3   | 1.71                     | 0.73              |
| 16:CQ:59:GLU:O     | 16:CQ:75:VAL:HG22  | 1.88                     | 0.73              |
| 23:DB:179:C:H5''   | 49:D2:28:ARG:NH1   | 2.04                     | 0.73              |
| 23:DB:2157:G:N3    | 23:DB:2157:G:H2'   | 2.04                     | 0.73              |
| 23:DB:2331:G:H4'   | 43:DW:69:GLU:HB2   | 1.71                     | 0.73              |
| 25:DC:68:ARG:NH2   | 25:DC:127:ASN:HA   | 2.02                     | 0.73              |
| 34:DM:92:TRP:HD1   | 34:DM:93:VAL:H     | 1.36                     | 0.73              |
| 36:DO:25:ARG:HE    | 36:DO:94:ARG:HH12  | 1.36                     | 0.73              |
| 1:AA:278:G:H21     | 1:AA:279:A:H62     | 1.36                     | 0.73              |
| 14:CO:88:ARG:HH22  | 23:DB:714:U:H3'    | 1.54                     | 0.73              |
| 23:DB:920:A:H2'    | 23:DB:921:C:H6     | 1.52                     | 0.73              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DB:1406:U:H2'   | 23:DB:1407:G:H8   | 1.53                     | 0.73              |
| 23:DB:2064:C:H2'   | 23:DB:2065:C:C6   | 2.24                     | 0.73              |
| 35:DN:34:ILE:HG22  | 35:DN:35:LYS:H    | 1.53                     | 0.73              |
| 42:DU:59:GLU:HG3   | 42:DU:62:ALA:HB2  | 1.69                     | 0.73              |
| 1:AA:239:U:OP1     | 1:AA:239:U:H4'    | 1.88                     | 0.73              |
| 1:AA:1026:G:H2'    | 1:AA:1027:C:C6    | 2.24                     | 0.73              |
| 11:AL:8:ARG:HG3    | 11:AL:9:LYS:N     | 2.00                     | 0.73              |
| 26:BD:159:LYS:HB2  | 26:BD:159:LYS:NZ  | 2.04                     | 0.73              |
| 34:BM:8:LYS:HE3    | 34:BM:70:ASP:HA   | 1.71                     | 0.73              |
| 13:CN:30:ILE:HG22  | 13:CN:41:TRP:HB3  | 1.70                     | 0.73              |
| 20:CB:59:ILE:HD12  | 20:CB:60:ALA:N    | 2.04                     | 0.73              |
| 22:DA:32:U:H1'     | 22:DA:52:A:N7     | 2.03                     | 0.73              |
| 23:DB:2684:U:H4'   | 32:DK:76:VAL:HG21 | 1.71                     | 0.73              |
| 27:DE:149:ILE:HG12 | 27:DE:186:VAL:HA  | 1.71                     | 0.73              |
| 28:DF:56:LEU:HA    | 28:DF:59:ILE:HG22 | 1.71                     | 0.73              |
| 34:DM:5:LYS:HB2    | 34:DM:69:PRO:HG2  | 1.71                     | 0.73              |
| 41:DT:67:VAL:HG12  | 41:DT:68:LYS:H    | 1.53                     | 0.73              |
| 42:DU:24:VAL:HG12  | 42:DU:26:ASN:OD1  | 1.87                     | 0.73              |
| 1:AA:812:G:N3      | 1:AA:812:G:H2'    | 2.02                     | 0.73              |
| 1:AA:1342:C:H2'    | 1:AA:1343:G:H8    | 1.54                     | 0.73              |
| 12:AM:11:HIS:N     | 12:AM:44:ILE:HD11 | 2.03                     | 0.73              |
| 18:AS:48:ILE:HB    | 18:AS:59:VAL:HB   | 1.71                     | 0.73              |
| 30:BH:73:ASN:HD22  | 30:BH:73:ASN:H    | 1.33                     | 0.73              |
| 51:B4:24:ARG:HH22  | 51:B4:36:ARG:HD2  | 1.54                     | 0.73              |
| 1:CA:278:G:H21     | 1:CA:279:A:H62    | 1.36                     | 0.73              |
| 1:CA:575:G:H4'     | 1:CA:576:C:O5'    | 1.87                     | 0.73              |
| 16:CQ:11:VAL:HG13  | 16:CQ:20:ILE:HG23 | 1.71                     | 0.73              |
| 20:CB:130:LYS:HB3  | 20:CB:134:LEU:HB2 | 1.70                     | 0.73              |
| 23:DB:1440:U:H2'   | 23:DB:1441:G:H8   | 1.51                     | 0.73              |
| 27:DE:49:ARG:HG3   | 27:DE:52:VAL:CG2  | 2.18                     | 0.73              |
| 29:DG:175:LYS:HG2  | 29:DG:176:LYS:H   | 1.54                     | 0.73              |
| 38:DQ:43:GLN:HA    | 39:DR:79:ARG:HG2  | 1.71                     | 0.73              |
| 52:DI:55:PRO:HD3   | 52:DI:74:PRO:HD3  | 1.69                     | 0.73              |
| 52:DI:72:THR:HG22  | 52:DI:115:ASP:OD2 | 1.89                     | 0.73              |
| 1:AA:1498:U:H3'    | 53:AA:1601:KSG:N1 | 2.04                     | 0.73              |
| 22:BA:20:G:H2'     | 22:BA:21:G:H8     | 1.54                     | 0.73              |
| 23:BB:222:A:N6     | 23:BB:232:G:H1'   | 2.03                     | 0.73              |
| 23:BB:704:G:O2'    | 23:BB:727:A:N6    | 2.22                     | 0.73              |
| 23:BB:934:U:H2'    | 23:BB:935:C:C6    | 2.24                     | 0.73              |
| 27:BE:195:GLN:H    | 27:BE:199:MET:HA  | 1.54                     | 0.73              |
| 34:BM:69:PRO:HB3   | 34:BM:93:VAL:HG12 | 1.70                     | 0.73              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 20:CB:99:MET:HA   | 20:CB:106:VAL:HG21 | 1.71                     | 0.73              |
| 23:DB:950:G:H2'   | 23:DB:951:C:C6     | 2.24                     | 0.73              |
| 23:DB:2814:A:H2'  | 23:DB:2815:C:H6    | 1.54                     | 0.73              |
| 34:DM:71:LYS:HZ3  | 34:DM:71:LYS:HA    | 1.53                     | 0.73              |
| 42:DU:38:ILE:HD13 | 42:DU:64:ILE:HG13  | 1.70                     | 0.73              |
| 45:DY:26:LEU:HD12 | 45:DY:28:LEU:HD22  | 1.70                     | 0.73              |
| 1:AA:982:U:H5''   | 13:AN:5:MET:HE2    | 1.71                     | 0.72              |
| 8:AI:117:LEU:HD22 | 8:AI:123:ARG:HG2   | 1.71                     | 0.72              |
| 22:BA:60:C:H2'    | 22:BA:61:G:C8      | 2.24                     | 0.72              |
| 23:BB:942:G:H5''  | 33:BL:40:SER:HB3   | 1.70                     | 0.72              |
| 23:BB:1041:G:H2'  | 23:BB:1042:G:H8    | 1.53                     | 0.72              |
| 25:BC:140:VAL:O   | 25:BC:141:HIS:HB2  | 1.89                     | 0.72              |
| 33:BL:79:LEU:HA   | 33:BL:113:ALA:HB3  | 1.71                     | 0.72              |
| 34:BM:4:PRO:HD3   | 34:BM:47:GLU:OE1   | 1.89                     | 0.72              |
| 34:BM:69:PRO:O    | 34:BM:70:ASP:HB3   | 1.86                     | 0.72              |
| 37:BP:27:VAL:HG21 | 37:BP:86:LYS:HB2   | 1.71                     | 0.72              |
| 1:CA:492:C:H2'    | 1:CA:493:A:H5''    | 1.71                     | 0.72              |
| 1:CA:1179:A:H2'   | 1:CA:1180:A:O4'    | 1.87                     | 0.72              |
| 11:CL:17:LYS:HB2  | 11:CL:17:LYS:NZ    | 2.04                     | 0.72              |
| 23:DB:1099:G:OP2  | 52:DI:3:LYS:HA     | 1.89                     | 0.72              |
| 23:DB:1241:A:H2'  | 23:DB:1242:U:H5'   | 1.69                     | 0.72              |
| 25:DC:141:HIS:HB3 | 25:DC:190:THR:HB   | 1.69                     | 0.72              |
| 33:DL:77:ILE:HD12 | 33:DL:77:ILE:N     | 2.03                     | 0.72              |
| 42:DU:4:ILE:HD13  | 42:DU:5:ARG:N      | 2.04                     | 0.72              |
| 42:DU:33:VAL:HG23 | 42:DU:65:GLN:NE2   | 2.04                     | 0.72              |
| 50:D3:51:LYS:HA   | 50:D3:51:LYS:NZ    | 2.03                     | 0.72              |
| 1:AA:922:G:H4'    | 4:AE:24:VAL:HA     | 1.70                     | 0.72              |
| 1:AA:927:G:H4'    | 1:AA:1503:A:N7     | 2.04                     | 0.72              |
| 2:AC:53:ARG:HG2   | 2:AC:54:ILE:H      | 1.54                     | 0.72              |
| 12:AM:18:LEU:HB3  | 12:AM:29:SER:HB2   | 1.69                     | 0.72              |
| 25:BC:79:ARG:NH1  | 25:BC:80:LEU:H     | 1.87                     | 0.72              |
| 4:CE:44:ARG:NH1   | 4:CE:72:ASN:HD21   | 1.86                     | 0.72              |
| 22:DA:51:G:C2'    | 22:DA:52:A:H5''    | 2.19                     | 0.72              |
| 23:DB:1714:U:H3'  | 23:DB:1715:G:C5'   | 2.18                     | 0.72              |
| 30:DH:39:ALA:O    | 30:DH:43:ASN:HB2   | 1.89                     | 0.72              |
| 38:DQ:69:ARG:HA   | 38:DQ:73:ILE:HG22  | 1.69                     | 0.72              |
| 39:DR:47:VAL:HG12 | 39:DR:49:ILE:HG12  | 1.71                     | 0.72              |
| 1:AA:78:A:H2'     | 1:AA:79:G:C8       | 2.24                     | 0.72              |
| 9:AJ:56:HIS:O     | 9:AJ:57:VAL:HG12   | 1.89                     | 0.72              |
| 23:BB:459:U:H5'   | 49:B2:41:ARG:HE    | 1.53                     | 0.72              |
| 23:BB:2722:G:H4'  | 35:BN:4:ARG:HB3    | 1.69                     | 0.72              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:BB:2895:G:H2'   | 23:BB:2896:C:C6   | 2.23                     | 0.72              |
| 41:BT:12:ARG:HE    | 44:BX:29:ARG:HH22 | 1.35                     | 0.72              |
| 1:CA:120:A:H2'     | 1:CA:121:U:H5''   | 1.71                     | 0.72              |
| 1:CA:1111:A:N1     | 2:CC:176:THR:HG22 | 2.03                     | 0.72              |
| 23:DB:151:C:H2'    | 23:DB:152:A:H8    | 1.52                     | 0.72              |
| 23:DB:1813:G:H21   | 25:DC:50:THR:HG23 | 1.55                     | 0.72              |
| 33:DL:92:LEU:HD22  | 33:DL:96:LYS:HG2  | 1.72                     | 0.72              |
| 41:DT:62:VAL:HG23  | 41:DT:63:VAL:H    | 1.55                     | 0.72              |
| 43:DW:69:GLU:HG3   | 43:DW:70:VAL:H    | 1.52                     | 0.72              |
| 1:AA:390:U:H2'     | 1:AA:391:G:C8     | 2.25                     | 0.72              |
| 1:AA:1062:U:H2'    | 1:AA:1063:C:C6    | 2.24                     | 0.72              |
| 22:BA:48:U:H2'     | 22:BA:49:C:C6     | 2.24                     | 0.72              |
| 29:BG:9:VAL:HG23   | 29:BG:47:ASN:HB3  | 1.70                     | 0.72              |
| 46:BZ:3:LYS:HE3    | 46:BZ:8:LYS:HA    | 1.69                     | 0.72              |
| 48:B1:14:ALA:HA    | 48:B1:48:TYR:HA   | 1.71                     | 0.72              |
| 1:CA:390:U:H2'     | 1:CA:391:G:C8     | 2.25                     | 0.72              |
| 5:CF:11:HIS:ND1    | 5:CF:12:PRO:HD2   | 2.04                     | 0.72              |
| 6:CG:90:VAL:HG13   | 6:CG:94:ARG:HD3   | 1.69                     | 0.72              |
| 13:CN:82:LYS:HE2   | 13:CN:85:GLU:HG3  | 1.71                     | 0.72              |
| 19:CT:38:ILE:HD11  | 19:CT:82:ILE:HG22 | 1.71                     | 0.72              |
| 23:DB:2471:A:O2'   | 23:DB:2472:G:H8   | 1.71                     | 0.72              |
| 27:DE:21:ARG:HH12  | 27:DE:23:PHE:HB3  | 1.55                     | 0.72              |
| 27:DE:153:LEU:HD13 | 27:DE:154:ASP:N   | 2.03                     | 0.72              |
| 47:D0:36:LYS:HB2   | 47:D0:41:HIS:HA   | 1.72                     | 0.72              |
| 52:DI:42:ASN:HA    | 52:DI:45:THR:OG1  | 1.90                     | 0.72              |
| 7:AH:76:ARG:HG2    | 7:AH:77:VAL:H     | 1.55                     | 0.72              |
| 23:BB:588:U:H5'    | 33:BL:28:GLY:HA2  | 1.71                     | 0.72              |
| 23:BB:616:A:H3'    | 23:BB:617:G:H8    | 1.54                     | 0.72              |
| 23:BB:811:U:H2'    | 33:BL:31:GLY:CA   | 2.18                     | 0.72              |
| 23:BB:1774:C:H2'   | 23:BB:1774:C:O2   | 1.88                     | 0.72              |
| 23:BB:2575:C:H5''  | 26:BD:149:ASN:CB  | 2.19                     | 0.72              |
| 1:CA:1060:U:H4'    | 9:CJ:54:SER:HB2   | 1.70                     | 0.72              |
| 6:CG:72:VAL:HG12   | 6:CG:89:GLU:HA    | 1.71                     | 0.72              |
| 13:CN:29:ILE:HG22  | 13:CN:30:ILE:HG13 | 1.71                     | 0.72              |
| 23:DB:974:G:H1'    | 23:DB:975:A:H8    | 1.54                     | 0.72              |
| 24:DV:7:GLU:HA     | 24:DV:65:VAL:HG23 | 1.71                     | 0.72              |
| 25:DC:143:VAL:HG12 | 25:DC:144:GLU:H   | 1.52                     | 0.72              |
| 1:AA:613:C:OP1     | 3:AD:80:ARG:HG3   | 1.90                     | 0.72              |
| 2:AC:26:LYS:HD3    | 2:AC:27:GLU:N     | 2.05                     | 0.72              |
| 23:BB:370:G:O2'    | 23:BB:423:A:H3'   | 1.89                     | 0.72              |
| 23:BB:1324:G:H1'   | 23:BB:1616:A:N6   | 2.05                     | 0.72              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:1406:U:H2'  | 23:BB:1407:G:H8    | 1.52                     | 0.72              |
| 23:BB:2064:C:H2'  | 23:BB:2065:C:H6    | 1.54                     | 0.72              |
| 24:BV:24:ASN:O    | 24:BV:44:HIS:HB2   | 1.89                     | 0.72              |
| 27:BE:98:LYS:HG3  | 27:BE:99:LYS:N     | 2.05                     | 0.72              |
| 31:BJ:20:ALA:HB1  | 31:BJ:59:ALA:HA    | 1.70                     | 0.72              |
| 33:BL:21:ARG:HB3  | 33:BL:21:ARG:NH1   | 2.04                     | 0.72              |
| 1:CA:269:C:H2'    | 1:CA:270:A:C8      | 2.24                     | 0.72              |
| 23:DB:1275:A:H2   | 23:DB:1645:G:H21   | 1.35                     | 0.72              |
| 27:DE:147:LEU:HB3 | 27:DE:167:VAL:HG13 | 1.71                     | 0.72              |
| 38:DQ:111:LYS:HE2 | 39:DR:52:PRO:HG3   | 1.71                     | 0.72              |
| 43:DW:58:LEU:HG   | 43:DW:81:ILE:HA    | 1.71                     | 0.72              |
| 50:D3:12:ARG:HB3  | 50:D3:23:HIS:CB    | 2.20                     | 0.72              |
| 1:AA:269:C:H2'    | 1:AA:270:A:C8      | 2.24                     | 0.72              |
| 4:AE:23:THR:HG23  | 4:AE:28:ARG:HD3    | 1.70                     | 0.72              |
| 23:BB:142:A:N3    | 41:BT:2:ILE:HD12   | 2.04                     | 0.72              |
| 23:BB:1224:U:H4'  | 39:BR:90:ARG:HB3   | 1.71                     | 0.72              |
| 23:BB:1275:A:H2   | 23:BB:1645:G:H21   | 1.35                     | 0.72              |
| 23:BB:2328:A:H2'  | 23:BB:2329:U:C6    | 2.24                     | 0.72              |
| 23:BB:2814:A:H2'  | 23:BB:2815:C:H6    | 1.54                     | 0.72              |
| 31:BJ:62:VAL:HG21 | 31:BJ:101:ILE:HD11 | 1.72                     | 0.72              |
| 32:BK:2:ILE:HD11  | 32:BK:8:LEU:HD11   | 1.71                     | 0.72              |
| 23:DB:414:C:H2'   | 23:DB:415:A:C8     | 2.24                     | 0.72              |
| 23:DB:2020:A:H5'  | 47:D0:8:THR:CG2    | 2.19                     | 0.72              |
| 23:DB:2091:C:H3'  | 23:DB:2092:U:C5'   | 2.19                     | 0.72              |
| 23:DB:2291:U:H2'  | 23:DB:2292:U:C6    | 2.25                     | 0.72              |
| 25:DC:63:ILE:HD12 | 25:DC:83:ASP:CG    | 2.15                     | 0.72              |
| 26:DD:61:THR:HG23 | 26:DD:62:LYS:HD3   | 1.70                     | 0.72              |
| 27:DE:130:LYS:HB2 | 27:DE:130:LYS:NZ   | 2.05                     | 0.72              |
| 35:DN:102:PHE:HD1 | 40:DS:40:ASN:HD21  | 1.37                     | 0.72              |
| 37:DP:49:ILE:O    | 37:DP:50:ARG:HD3   | 1.89                     | 0.72              |
| 6:AG:148:LYS:HG3  | 6:AG:151:ALA:HB3   | 1.71                     | 0.72              |
| 9:AJ:67:ILE:HG13  | 13:AN:95:LEU:HD13  | 1.71                     | 0.72              |
| 13:AN:60:ARG:HH21 | 13:AN:62:ARG:HE    | 1.36                     | 0.72              |
| 23:BB:155:A:H2'   | 23:BB:156:A:C8     | 2.24                     | 0.72              |
| 23:BB:2241:A:H2'  | 23:BB:2242:G:C8    | 2.25                     | 0.72              |
| 26:BD:106:LYS:NZ  | 26:BD:208:LYS:HD3  | 2.04                     | 0.72              |
| 27:BE:147:LEU:O   | 27:BE:148:ILE:HG13 | 1.90                     | 0.72              |
| 34:BM:3:GLN:HG2   | 34:BM:46:ILE:HB    | 1.70                     | 0.72              |
| 37:BP:26:GLU:HA   | 37:BP:46:VAL:HG13  | 1.71                     | 0.72              |
| 46:BZ:8:LYS:CD    | 46:BZ:9:TYR:H      | 2.01                     | 0.72              |
| 1:CA:1000:A:H2'   | 1:CA:1001:C:C6     | 2.23                     | 0.72              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 14:CO:38:LEU:HD23 | 14:CO:55:LEU:HD13  | 1.72                     | 0.72              |
| 16:CQ:68:LYS:HG2  | 16:CQ:69:THR:HG23  | 1.72                     | 0.72              |
| 23:DB:833:A:H1'   | 33:DL:54:GLN:OE1   | 1.89                     | 0.72              |
| 23:DB:836:G:H2'   | 23:DB:837:C:C6     | 2.24                     | 0.72              |
| 23:DB:1774:C:H2'  | 23:DB:1774:C:O2    | 1.88                     | 0.72              |
| 23:DB:2898:U:O2'  | 31:DJ:137:PRO:HB3  | 1.89                     | 0.72              |
| 25:DC:10:PRO:HD2  | 25:DC:202:ARG:HH22 | 1.53                     | 0.72              |
| 33:DL:77:ILE:HD12 | 33:DL:77:ILE:H     | 1.54                     | 0.72              |
| 35:DN:56:LYS:HG3  | 35:DN:57:THR:H     | 1.55                     | 0.72              |
| 1:AA:95:C:O2      | 1:AA:95:C:H2'      | 1.87                     | 0.72              |
| 1:AA:859:G:H2'    | 1:AA:860:A:C8      | 2.25                     | 0.72              |
| 1:AA:1308:U:H2'   | 1:AA:1309:G:H8     | 1.55                     | 0.72              |
| 13:AN:12:ARG:HA   | 13:AN:15:LEU:HD11  | 1.71                     | 0.72              |
| 23:BB:136:G:H2'   | 23:BB:137:U:C6     | 2.25                     | 0.72              |
| 23:BB:1275:A:H3'  | 23:BB:1275:A:N3    | 2.05                     | 0.72              |
| 35:BN:28:LEU:HD11 | 35:BN:44:LEU:HD21  | 1.72                     | 0.72              |
| 1:CA:439:U:H4'    | 3:CD:120:LYS:HD2   | 1.72                     | 0.72              |
| 23:DB:1309:G:H5'' | 49:D2:9:VAL:HG13   | 1.72                     | 0.72              |
| 28:DF:45:ASP:O    | 28:DF:46:LYS:HG3   | 1.90                     | 0.72              |
| 35:DN:28:LEU:HA   | 35:DN:34:ILE:HD11  | 1.72                     | 0.72              |
| 1:AA:1035:A:H2'   | 1:AA:1036:A:H8     | 1.53                     | 0.72              |
| 6:AG:94:ARG:HD3   | 6:AG:98:LEU:HD11   | 1.72                     | 0.72              |
| 23:BB:324:A:H2'   | 23:BB:325:G:O4'    | 1.89                     | 0.72              |
| 27:BE:44:ARG:HD3  | 27:BE:44:ARG:H     | 1.53                     | 0.72              |
| 33:BL:30:THR:HA   | 33:BL:36:LYS:HE3   | 1.71                     | 0.72              |
| 2:CC:128:MET:SD   | 2:CC:131:ARG:HB2   | 2.29                     | 0.72              |
| 4:CE:23:THR:HA    | 4:CE:28:ARG:HA     | 1.72                     | 0.72              |
| 4:CE:104:ILE:HD12 | 4:CE:111:ARG:HD3   | 1.72                     | 0.72              |
| 6:CG:12:LEU:HD22  | 6:CG:13:PRO:HD2    | 1.72                     | 0.72              |
| 23:DB:1469:A:H2'  | 23:DB:1470:A:C8    | 2.25                     | 0.72              |
| 23:DB:2328:A:H2'  | 23:DB:2329:U:C6    | 2.24                     | 0.72              |
| 25:DC:26:GLY:C    | 25:DC:27:LYS:HD2   | 2.15                     | 0.72              |
| 33:DL:109:LYS:HE2 | 33:DL:126:ARG:CZ   | 2.20                     | 0.72              |
| 36:DO:25:ARG:HG2  | 36:DO:94:ARG:HH22  | 1.54                     | 0.72              |
| 36:DO:28:VAL:HG13 | 36:DO:106:LEU:HD13 | 1.72                     | 0.72              |
| 38:DQ:69:ARG:HB3  | 38:DQ:69:ARG:NH1   | 2.05                     | 0.72              |
| 40:DS:42:LYS:O    | 40:DS:45:VAL:HG13  | 1.90                     | 0.72              |
| 43:DW:43:LYS:O    | 43:DW:44:PHE:HB2   | 1.87                     | 0.72              |
| 1:AA:275:G:C5'    | 16:AQ:15:LYS:HG2   | 2.20                     | 0.71              |
| 2:AC:13:ILE:O     | 2:AC:14:VAL:HG22   | 1.90                     | 0.71              |
| 5:AF:54:LEU:HD13  | 5:AF:55:HIS:H      | 1.55                     | 0.71              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:AH:49:LYS:HG3    | 7:AH:50:VAL:H      | 1.55                     | 0.71              |
| 23:BB:2246:G:H2'   | 23:BB:2247:A:H8    | 1.55                     | 0.71              |
| 23:BB:2266:A:C4'   | 23:BB:2267:A:N7    | 2.53                     | 0.71              |
| 26:BD:175:LEU:HD11 | 26:BD:192:ALA:HB3  | 1.72                     | 0.71              |
| 27:BE:159:LEU:HA   | 27:BE:169:VAL:HG21 | 1.71                     | 0.71              |
| 30:BH:57:LYS:HG3   | 30:BH:61:VAL:HG21  | 1.70                     | 0.71              |
| 34:BM:37:GLY:H     | 34:BM:97:GLN:HE21  | 1.35                     | 0.71              |
| 42:BU:60:LYS:HG3   | 42:BU:61:GLU:H     | 1.54                     | 0.71              |
| 1:CA:1289:A:H3'    | 1:CA:1290:G:H8     | 1.55                     | 0.71              |
| 8:CI:79:ARG:O      | 8:CI:79:ARG:HD2    | 1.90                     | 0.71              |
| 23:DB:289:G:H2'    | 23:DB:290:U:C6     | 2.24                     | 0.71              |
| 23:DB:598:U:H5'    | 33:DL:21:ARG:HB2   | 1.70                     | 0.71              |
| 23:DB:1118:C:H2'   | 23:DB:1119:U:H6    | 1.54                     | 0.71              |
| 23:DB:1275:A:H3'   | 23:DB:1275:A:N3    | 2.05                     | 0.71              |
| 23:DB:1429:G:H2'   | 23:DB:1430:G:H8    | 1.55                     | 0.71              |
| 25:DC:28:PRO:HG2   | 25:DC:79:ARG:CZ    | 2.20                     | 0.71              |
| 39:DR:65:ALA:HB3   | 39:DR:100:GLY:H    | 1.55                     | 0.71              |
| 1:AA:545:C:O2'     | 1:AA:546:A:H5'     | 1.90                     | 0.71              |
| 1:AA:1060:U:H5''   | 9:AJ:53:ILE:HG22   | 1.71                     | 0.71              |
| 4:AE:105:ILE:HB    | 4:AE:123:LEU:HA    | 1.70                     | 0.71              |
| 20:AB:67:LEU:HD22  | 20:AB:67:LEU:H     | 1.54                     | 0.71              |
| 23:BB:532:A:H4'    | 23:BB:533:G:C8     | 2.25                     | 0.71              |
| 23:BB:2147:A:C5'   | 23:BB:2148:G:H5'   | 2.19                     | 0.71              |
| 23:BB:2331:G:H4'   | 43:BW:69:GLU:HG2   | 1.70                     | 0.71              |
| 23:BB:2461:A:H2'   | 23:BB:2462:C:C6    | 2.24                     | 0.71              |
| 30:BH:8:LYS:HD3    | 30:BH:8:LYS:O      | 1.90                     | 0.71              |
| 31:BJ:71:ASP:CG    | 31:BJ:72:LYS:N     | 2.47                     | 0.71              |
| 39:BR:6:GLN:HG2    | 39:BR:10:LYS:HE2   | 1.72                     | 0.71              |
| 41:BT:54:GLU:H     | 41:BT:91:GLN:NE2   | 1.86                     | 0.71              |
| 1:CA:1361:G:H2'    | 1:CA:1362:A:H5''   | 1.73                     | 0.71              |
| 13:CN:73:LEU:HD12  | 13:CN:83:VAL:HG21  | 1.70                     | 0.71              |
| 23:DB:2039:U:H2'   | 23:DB:2040:G:H8    | 1.56                     | 0.71              |
| 1:AA:120:A:H2'     | 1:AA:121:U:H5''    | 1.70                     | 0.71              |
| 23:BB:543:G:C2'    | 23:BB:544:C:H5''   | 2.19                     | 0.71              |
| 25:BC:20:ASN:HB2   | 25:BC:203:VAL:HG13 | 1.72                     | 0.71              |
| 26:BD:52:THR:HG22  | 26:BD:75:ALA:HB1   | 1.73                     | 0.71              |
| 29:BG:175:LYS:HD3  | 29:BG:176:LYS:HB2  | 1.72                     | 0.71              |
| 48:B1:31:GLU:HG3   | 48:B1:32:LYS:H     | 1.54                     | 0.71              |
| 50:B3:24:LYS:HZ1   | 50:B3:29:ARG:HH12  | 1.35                     | 0.71              |
| 51:B4:25:VAL:HB    | 51:B4:33:HIS:O     | 1.90                     | 0.71              |
| 52:BI:89:SER:HA    | 52:BI:97:VAL:HG21  | 1.72                     | 0.71              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:CL:98:ARG:HB3  | 11:CL:116:TYR:HA   | 1.71                     | 0.71              |
| 23:DB:643:A:H61   | 23:DB:2370:G:H1'   | 1.55                     | 0.71              |
| 23:DB:1175:A:C2'  | 23:DB:1176:U:H5'   | 2.19                     | 0.71              |
| 23:DB:2461:A:H2'  | 23:DB:2462:C:C6    | 2.25                     | 0.71              |
| 25:DC:68:ARG:HH22 | 25:DC:127:ASN:HA   | 1.54                     | 0.71              |
| 28:DF:7:TYR:O     | 28:DF:11:VAL:HB    | 1.90                     | 0.71              |
| 39:DR:18:GLN:HA   | 39:DR:99:THR:HA    | 1.73                     | 0.71              |
| 3:AD:154:VAL:HG13 | 3:AD:155:LYS:H     | 1.55                     | 0.71              |
| 20:AB:41:ASN:HD22 | 20:AB:44:LYS:HB2   | 1.53                     | 0.71              |
| 26:BD:128:ARG:HA  | 26:BD:128:ARG:HE   | 1.55                     | 0.71              |
| 33:BL:78:ARG:H    | 33:BL:110:VAL:HG13 | 1.55                     | 0.71              |
| 1:CA:559:A:H4'    | 1:CA:560:A:H3'     | 1.73                     | 0.71              |
| 3:CD:63:ILE:HG23  | 3:CD:64:TYR:CD1    | 2.24                     | 0.71              |
| 21:CU:15:LEU:HA   | 21:CU:17:ARG:HH11  | 1.56                     | 0.71              |
| 22:DA:76:G:H2'    | 22:DA:77:U:H6      | 1.54                     | 0.71              |
| 23:DB:11:C:H2'    | 23:DB:12:U:H5'     | 1.72                     | 0.71              |
| 23:DB:438:G:H2'   | 23:DB:439:A:H8     | 1.56                     | 0.71              |
| 23:DB:448:U:H3'   | 27:DE:79:ARG:HH21  | 1.55                     | 0.71              |
| 23:DB:483:A:H2'   | 23:DB:484:C:H5'    | 1.70                     | 0.71              |
| 23:DB:856:G:C4'   | 43:DW:23:LYS:HD2   | 2.19                     | 0.71              |
| 23:DB:2784:U:H4'  | 26:DD:42:ASN:H     | 1.54                     | 0.71              |
| 26:DD:37:VAL:HG11 | 26:DD:46:ARG:HD3   | 1.72                     | 0.71              |
| 52:DI:73:PRO:HG2  | 52:DI:78:LEU:HD21  | 1.72                     | 0.71              |
| 1:AA:275:G:H5'    | 16:AQ:15:LYS:HG2   | 1.72                     | 0.71              |
| 1:AA:1049:U:H2'   | 13:AN:2:LYS:HD3    | 1.70                     | 0.71              |
| 23:BB:1395:A:H4'  | 23:BB:1397:U:C5    | 2.26                     | 0.71              |
| 23:BB:1797:G:O3'  | 25:BC:253:GLY:HA2  | 1.91                     | 0.71              |
| 28:BF:12:VAL:HG13 | 28:BF:27:VAL:HG11  | 1.71                     | 0.71              |
| 33:BL:60:ARG:HA   | 33:BL:60:ARG:NH1   | 2.06                     | 0.71              |
| 41:BT:88:LYS:HG2  | 41:BT:89:GLU:N     | 2.04                     | 0.71              |
| 45:BY:9:THR:HG23  | 45:BY:10:ARG:H     | 1.55                     | 0.71              |
| 50:B3:44:ARG:HG3  | 50:B3:45:PRO:HD2   | 1.73                     | 0.71              |
| 1:CA:8:A:H1'      | 4:CE:107:GLY:HA2   | 1.71                     | 0.71              |
| 1:CA:84:U:O2'     | 1:CA:85:U:H5'      | 1.89                     | 0.71              |
| 1:CA:1009:U:H1'   | 1:CA:1021:A:N1     | 2.05                     | 0.71              |
| 5:CF:38:ARG:HH21  | 5:CF:63:ASN:ND2    | 1.88                     | 0.71              |
| 6:CG:14:ASP:HB3   | 6:CG:18:GLY:N      | 2.06                     | 0.71              |
| 9:CJ:66:GLU:HB2   | 13:CN:98:ALA:HB2   | 1.72                     | 0.71              |
| 17:CR:51:GLN:HA   | 17:CR:54:LEU:HD13  | 1.71                     | 0.71              |
| 21:CU:14:ALA:H    | 21:CU:16:ARG:NH2   | 1.89                     | 0.71              |
| 23:DB:480:A:O4'   | 42:DU:40:LEU:HD22  | 1.89                     | 0.71              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DB:1060:U:C4    | 23:DB:1088:A:N6   | 2.58                     | 0.71              |
| 23:DB:1395:A:H4'   | 23:DB:1397:U:C5   | 2.26                     | 0.71              |
| 25:DC:127:ASN:HD22 | 25:DC:128:THR:N   | 1.87                     | 0.71              |
| 26:DD:6:GLY:HA2    | 26:DD:199:SER:O   | 1.90                     | 0.71              |
| 33:DL:77:ILE:HD13  | 33:DL:110:VAL:N   | 2.05                     | 0.71              |
| 38:DQ:46:TYR:HA    | 39:DR:77:PHE:HD2  | 1.56                     | 0.71              |
| 45:DY:3:THR:HA     | 45:DY:37:ARG:H    | 1.56                     | 0.71              |
| 1:AA:8:A:H2'       | 3:AD:205:LYS:O    | 1.91                     | 0.71              |
| 1:AA:492:C:H2'     | 1:AA:493:A:H5''   | 1.71                     | 0.71              |
| 1:AA:1208:C:H2'    | 1:AA:1209:C:O4'   | 1.91                     | 0.71              |
| 25:BC:28:PRO:O     | 25:BC:29:PHE:HB3  | 1.90                     | 0.71              |
| 29:BG:94:ARG:HH11  | 29:BG:94:ARG:HB2  | 1.55                     | 0.71              |
| 29:BG:176:LYS:HE2  | 29:BG:176:LYS:C   | 2.15                     | 0.71              |
| 39:BR:74:ILE:HA    | 39:BR:90:ARG:NE   | 2.03                     | 0.71              |
| 49:B2:13:ASN:HB2   | 49:B2:18:PHE:HD2  | 1.56                     | 0.71              |
| 23:DB:363:G:H2'    | 23:DB:364:C:C6    | 2.25                     | 0.71              |
| 23:DB:616:A:H3'    | 23:DB:617:G:H8    | 1.54                     | 0.71              |
| 23:DB:1324:G:H1'   | 23:DB:1616:A:N6   | 2.05                     | 0.71              |
| 26:DD:125:TRP:HD1  | 26:DD:127:PHE:HB2 | 1.56                     | 0.71              |
| 37:DP:55:HIS:C     | 37:DP:57:ALA:H    | 1.96                     | 0.71              |
| 1:AA:17:U:H2'      | 1:AA:18:C:H6      | 1.55                     | 0.71              |
| 1:AA:188:C:H2'     | 1:AA:189:A:O4'    | 1.90                     | 0.71              |
| 1:AA:559:A:H4'     | 1:AA:560:A:H3'    | 1.73                     | 0.71              |
| 1:AA:1250:A:H4'    | 8:AI:69:GLY:H     | 1.56                     | 0.71              |
| 1:AA:1284:C:H3'    | 1:AA:1285:A:H5''  | 1.72                     | 0.71              |
| 6:AG:38:ALA:O      | 6:AG:41:ILE:HG22  | 1.91                     | 0.71              |
| 10:AK:42:GLY:HA3   | 10:AK:73:VAL:HG22 | 1.71                     | 0.71              |
| 12:AM:64:VAL:HG12  | 12:AM:65:GLU:H    | 1.54                     | 0.71              |
| 22:BA:48:U:H2'     | 22:BA:49:C:H6     | 1.56                     | 0.71              |
| 23:BB:1041:G:H2'   | 23:BB:1042:G:C8   | 2.25                     | 0.71              |
| 23:BB:1173:U:C4    | 23:BB:1174:U:H1'  | 2.26                     | 0.71              |
| 23:BB:1429:G:H2'   | 23:BB:1430:G:H8   | 1.55                     | 0.71              |
| 26:BD:31:ALA:HB1   | 26:BD:49:GLN:HG3  | 1.73                     | 0.71              |
| 28:BF:31:GLU:H     | 28:BF:157:THR:HA  | 1.54                     | 0.71              |
| 33:BL:100:ILE:HG12 | 33:BL:102:GLY:H   | 1.55                     | 0.71              |
| 35:BN:35:LYS:HA    | 35:BN:111:ALA:O   | 1.91                     | 0.71              |
| 43:BW:19:ARG:NH2   | 43:BW:71:LYS:HD3  | 2.06                     | 0.71              |
| 51:B4:7:VAL:HG12   | 51:B4:8:LYS:H     | 1.54                     | 0.71              |
| 51:B4:33:HIS:H     | 51:B4:33:HIS:CD2  | 2.07                     | 0.71              |
| 3:CD:101:VAL:HG13  | 3:CD:106:PHE:HD2  | 1.54                     | 0.71              |
| 19:CT:19:HIS:O     | 19:CT:23:ARG:HG2  | 1.91                     | 0.71              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:455:C:N3    | 23:DB:472:A:H2'    | 2.06                     | 0.71              |
| 23:DB:1080:A:H2'  | 23:DB:1081:U:C6    | 2.25                     | 0.71              |
| 23:DB:1700:A:H2'  | 23:DB:1701:A:H5'   | 1.72                     | 0.71              |
| 28:DF:31:GLU:HG3  | 28:DF:158:THR:HG22 | 1.71                     | 0.71              |
| 28:DF:59:ILE:HD13 | 28:DF:59:ILE:O     | 1.90                     | 0.71              |
| 40:DS:74:ILE:HG22 | 40:DS:105:VAL:HG23 | 1.72                     | 0.71              |
| 41:DT:49:LYS:O    | 41:DT:50:LEU:HG    | 1.90                     | 0.71              |
| 50:D3:4:LYS:HD2   | 50:D3:59:ALA:HA    | 1.72                     | 0.71              |
| 8:AI:23:GLY:H     | 8:AI:60:LEU:HA     | 1.54                     | 0.71              |
| 12:AM:21:ILE:HG22 | 12:AM:64:VAL:HG11  | 1.72                     | 0.71              |
| 23:BB:452:G:OP1   | 27:BE:52:VAL:HG22  | 1.90                     | 0.71              |
| 23:BB:1439:A:N1   | 23:BB:1552:A:N7    | 2.39                     | 0.71              |
| 23:BB:2575:C:C5'  | 26:BD:149:ASN:H    | 2.04                     | 0.71              |
| 25:BC:107:LYS:HB2 | 25:BC:194:VAL:CG1  | 2.20                     | 0.71              |
| 33:BL:13:LYS:HG3  | 33:BL:14:LYS:N     | 2.01                     | 0.71              |
| 37:BP:29:VAL:HG22 | 37:BP:47:ILE:HD11  | 1.72                     | 0.71              |
| 38:BQ:93:ILE:HG23 | 38:BQ:94:LEU:H     | 1.55                     | 0.71              |
| 41:BT:93:LEU:HD22 | 41:BT:93:LEU:H     | 1.56                     | 0.71              |
| 5:CF:79:ARG:HH22  | 5:CF:87:SER:HB3    | 1.56                     | 0.71              |
| 20:CB:62:ARG:HD2  | 20:CB:62:ARG:H     | 1.56                     | 0.71              |
| 20:CB:139:GLU:O   | 20:CB:143:LEU:HB2  | 1.91                     | 0.71              |
| 23:DB:242:G:N2    | 23:DB:254:G:H2'    | 2.06                     | 0.71              |
| 23:DB:380:G:O2'   | 46:DZ:13:THR:HB    | 1.90                     | 0.71              |
| 23:DB:972:A:C3'   | 23:DB:973:A:H5''   | 2.21                     | 0.71              |
| 40:DS:17:VAL:O    | 40:DS:20:VAL:HG12  | 1.90                     | 0.71              |
| 41:DT:29:THR:HB   | 41:DT:86:THR:HA    | 1.72                     | 0.71              |
| 50:D3:4:LYS:NZ    | 50:D3:60:CYS:H     | 1.89                     | 0.71              |
| 1:AA:279:A:H5''   | 1:AA:280:C:H3'     | 1.72                     | 0.71              |
| 23:BB:1203:U:H3'  | 23:BB:1204:A:H5''  | 1.71                     | 0.71              |
| 23:BB:1813:G:H21  | 25:BC:51:ARG:CG    | 2.04                     | 0.71              |
| 23:BB:1951:U:H2'  | 23:BB:1953:A:OP2   | 1.91                     | 0.71              |
| 23:BB:2393:U:H5'  | 33:BL:62:PRO:HD3   | 1.73                     | 0.71              |
| 33:BL:60:ARG:HH11 | 50:B3:11:LYS:HE2   | 1.53                     | 0.71              |
| 1:CA:560:A:H5'    | 1:CA:566:G:N2      | 2.05                     | 0.71              |
| 1:CA:859:G:H2'    | 1:CA:860:A:C8      | 2.25                     | 0.71              |
| 1:CA:1097:C:H2'   | 1:CA:1098:C:C6     | 2.26                     | 0.71              |
| 1:CA:1218:C:H2'   | 1:CA:1219:A:C8     | 2.26                     | 0.71              |
| 23:DB:1028:A:H2'  | 23:DB:1029:A:C8    | 2.26                     | 0.71              |
| 23:DB:1098:A:H3'  | 52:DI:3:LYS:C      | 2.15                     | 0.71              |
| 23:DB:1439:A:N1   | 23:DB:1552:A:N7    | 2.39                     | 0.71              |
| 23:DB:2874:C:OP1  | 35:DN:5:LYS:HD2    | 1.91                     | 0.71              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:DS:23:LEU:C    | 40:DS:24:ILE:HD13  | 2.15                     | 0.71              |
| 41:DT:60:THR:HA   | 41:DT:82:LYS:O     | 1.90                     | 0.71              |
| 45:DY:40:THR:HG23 | 45:DY:43:ILE:HG22  | 1.73                     | 0.71              |
| 4:AE:155:LYS:HG3  | 7:AH:65:PHE:HB2    | 1.73                     | 0.71              |
| 15:AP:20:VAL:HG23 | 15:AP:35:ARG:HA    | 1.71                     | 0.71              |
| 23:BB:414:C:H2'   | 23:BB:415:A:C8     | 2.25                     | 0.71              |
| 23:BB:1060:U:C4   | 23:BB:1088:A:N6    | 2.58                     | 0.71              |
| 23:BB:1485:U:H2'  | 23:BB:1486:U:C6    | 2.26                     | 0.71              |
| 23:BB:1700:A:H2'  | 23:BB:1701:A:H5'   | 1.72                     | 0.71              |
| 23:BB:2039:U:H2'  | 23:BB:2040:G:H8    | 1.56                     | 0.71              |
| 25:BC:68:ARG:HD3  | 25:BC:103:ILE:HD11 | 1.72                     | 0.71              |
| 29:BG:71:LEU:HA   | 29:BG:74:MET:SD    | 2.31                     | 0.71              |
| 31:BJ:99:ARG:HA   | 31:BJ:103:ILE:HG13 | 1.73                     | 0.71              |
| 33:BL:78:ARG:NH2  | 33:BL:82:LEU:HB2   | 2.06                     | 0.71              |
| 36:BO:21:LEU:O    | 36:BO:42:PRO:HB3   | 1.91                     | 0.71              |
| 36:BO:48:LEU:HD23 | 36:BO:49:VAL:N     | 2.06                     | 0.71              |
| 47:B0:29:VAL:HB   | 47:B0:36:LYS:HD2   | 1.73                     | 0.71              |
| 3:CD:34:GLU:O     | 3:CD:35:GLN:HG3    | 1.91                     | 0.71              |
| 9:CJ:32:THR:HG23  | 9:CJ:33:GLY:H      | 1.56                     | 0.71              |
| 23:DB:96:C:H4'    | 44:DX:41:HIS:CE1   | 2.26                     | 0.71              |
| 23:DB:860:U:O2'   | 23:DB:2267:A:H4'   | 1.91                     | 0.71              |
| 23:DB:950:G:H2'   | 23:DB:951:C:H6     | 1.54                     | 0.71              |
| 23:DB:1594:U:H2'  | 23:DB:1595:C:C6    | 2.25                     | 0.71              |
| 29:DG:39:ALA:HB1  | 29:DG:54:ARG:H     | 1.56                     | 0.71              |
| 30:DH:94:ILE:HG23 | 30:DH:98:ASP:CB    | 2.20                     | 0.71              |
| 43:DW:66:VAL:HG22 | 43:DW:67:LYS:N     | 2.06                     | 0.71              |
| 3:AD:10:LEU:HD21  | 3:AD:62:ARG:HD3    | 1.73                     | 0.70              |
| 15:AP:51:ARG:C    | 15:AP:52:LEU:HD22  | 2.16                     | 0.70              |
| 20:AB:69:VAL:O    | 20:AB:163:ILE:HG22 | 1.91                     | 0.70              |
| 22:BA:49:C:H2'    | 22:BA:50:A:C8      | 2.26                     | 0.70              |
| 23:BB:279:A:H61   | 23:BB:361:G:H1'    | 1.54                     | 0.70              |
| 23:BB:2037:A:H2'  | 23:BB:2038:G:C8    | 2.26                     | 0.70              |
| 23:BB:2041:U:H2'  | 23:BB:2042:A:C8    | 2.25                     | 0.70              |
| 23:BB:2147:A:H5'  | 23:BB:2148:G:C5'   | 2.20                     | 0.70              |
| 23:BB:2537:U:H2'  | 23:BB:2538:C:C6    | 2.25                     | 0.70              |
| 25:BC:87:SER:O    | 25:BC:157:ALA:HB2  | 1.90                     | 0.70              |
| 27:BE:151:GLY:O   | 27:BE:190:ALA:HB2  | 1.90                     | 0.70              |
| 36:BO:16:ARG:HA   | 36:BO:16:ARG:NE    | 2.06                     | 0.70              |
| 40:BS:28:LYS:HD3  | 40:BS:71:VAL:HG21  | 1.72                     | 0.70              |
| 43:BW:46:ALA:H    | 43:BW:75:ASN:CG    | 1.99                     | 0.70              |
| 1:CA:764:C:H3'    | 1:CA:765:G:N2      | 2.06                     | 0.70              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:CH:31:LEU:HG     | 7:CH:35:ILE:HD11   | 1.73                     | 0.70              |
| 10:CK:12:ARG:C     | 10:CK:13:LYS:HD2   | 2.15                     | 0.70              |
| 23:DB:864:G:O2'    | 23:DB:865:C:H5'    | 1.91                     | 0.70              |
| 23:DB:1203:U:H3'   | 23:DB:1204:A:H5''  | 1.73                     | 0.70              |
| 39:DR:79:ARG:HD3   | 39:DR:81:LYS:HG3   | 1.72                     | 0.70              |
| 51:D4:34:LYS:HE2   | 51:D4:36:ARG:HH22  | 1.55                     | 0.70              |
| 1:AA:560:A:H5'     | 1:AA:566:G:N2      | 2.06                     | 0.70              |
| 1:AA:878:A:H5''    | 7:AH:80:PRO:HG2    | 1.74                     | 0.70              |
| 1:AA:1241:G:H2'    | 1:AA:1242:G:H8     | 1.57                     | 0.70              |
| 2:AC:69:THR:HG21   | 2:AC:75:VAL:HG21   | 1.73                     | 0.70              |
| 4:AE:114:LEU:HD22  | 4:AE:119:VAL:HG21  | 1.73                     | 0.70              |
| 23:BB:855:G:H21    | 43:BW:23:LYS:CB    | 2.03                     | 0.70              |
| 23:BB:1060:U:C5    | 52:BI:131:THR:HG22 | 2.25                     | 0.70              |
| 23:BB:1469:A:H2'   | 23:BB:1470:A:C8    | 2.25                     | 0.70              |
| 30:BH:90:LEU:HD21  | 30:BH:146:VAL:HG11 | 1.72                     | 0.70              |
| 34:BM:73:ILE:HD13  | 34:BM:92:TRP:H     | 1.56                     | 0.70              |
| 41:BT:61:LEU:HD12  | 41:BT:62:VAL:H     | 1.56                     | 0.70              |
| 52:BI:89:SER:HB2   | 52:BI:136:GLY:HA3  | 1.73                     | 0.70              |
| 3:CD:187:ARG:HH12  | 3:CD:191:SER:HA    | 1.55                     | 0.70              |
| 4:CE:87:VAL:HG22   | 4:CE:88:HIS:H      | 1.55                     | 0.70              |
| 13:CN:51:PRO:HG2   | 13:CN:52:ARG:H     | 1.56                     | 0.70              |
| 23:DB:28:A:N6      | 23:DB:512:G:O2'    | 2.24                     | 0.70              |
| 23:DB:350:G:H2'    | 23:DB:351:C:O4'    | 1.91                     | 0.70              |
| 23:DB:2306:C:H3'   | 23:DB:2307:G:H5''  | 1.72                     | 0.70              |
| 31:DJ:35:ARG:HB3   | 31:DJ:54:ILE:HD11  | 1.72                     | 0.70              |
| 41:DT:72:GLN:C     | 41:DT:73:ARG:HD2   | 2.16                     | 0.70              |
| 42:DU:43:LYS:HG2   | 42:DU:57:ILE:HB    | 1.73                     | 0.70              |
| 5:AF:53:LYS:HD3    | 5:AF:54:LEU:N      | 2.04                     | 0.70              |
| 23:BB:131:A:H2'    | 23:BB:132:G:H8     | 1.57                     | 0.70              |
| 23:BB:1182:G:H2'   | 23:BB:1183:U:O4'   | 1.90                     | 0.70              |
| 23:BB:2197:U:O2'   | 23:BB:2198:A:H2'   | 1.91                     | 0.70              |
| 23:BB:2483:C:H4'   | 34:BM:51:ARG:HH12  | 1.56                     | 0.70              |
| 25:BC:10:PRO:HD2   | 25:BC:202:ARG:HH12 | 1.57                     | 0.70              |
| 1:CA:451:A:H4'     | 1:CA:452:A:O4'     | 1.91                     | 0.70              |
| 1:CA:1238:A:H5'    | 1:CA:1336:C:N4     | 2.04                     | 0.70              |
| 12:CM:52:ILE:HA    | 12:CM:55:LEU:HD12  | 1.72                     | 0.70              |
| 23:DB:1951:U:H2'   | 23:DB:1953:A:OP2   | 1.91                     | 0.70              |
| 23:DB:2037:A:H2'   | 23:DB:2038:G:C8    | 2.26                     | 0.70              |
| 23:DB:2557:G:H2'   | 23:DB:2558:C:C6    | 2.27                     | 0.70              |
| 25:DC:164:VAL:HG23 | 25:DC:167:ASP:HB2  | 1.71                     | 0.70              |
| 26:DD:61:THR:HG23  | 26:DD:62:LYS:H     | 1.54                     | 0.70              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 43:DW:42:THR:H    | 43:DW:65:LYS:HG2   | 1.57                     | 0.70              |
| 48:D1:40:PRO:HD2  | 48:D1:44:GLN:O     | 1.90                     | 0.70              |
| 51:D4:30:GLU:HB3  | 51:D4:33:HIS:HB2   | 1.72                     | 0.70              |
| 4:AE:101:GLY:H    | 4:AE:121:ASN:HD21  | 1.39                     | 0.70              |
| 23:BB:287:G:H2'   | 23:BB:288:U:H6     | 1.55                     | 0.70              |
| 23:BB:1082:U:C4   | 23:BB:1086:A:C2    | 2.80                     | 0.70              |
| 23:BB:2228:G:H2'  | 23:BB:2229:U:C6    | 2.26                     | 0.70              |
| 29:BG:19:ASN:HB3  | 29:BG:22:VAL:HG13  | 1.72                     | 0.70              |
| 29:BG:40:VAL:HB   | 29:BG:63:GLN:HE22  | 1.57                     | 0.70              |
| 31:BJ:41:LYS:HD2  | 31:BJ:44:TYR:HB2   | 1.73                     | 0.70              |
| 34:BM:33:LEU:N    | 34:BM:101:VAL:HG22 | 2.06                     | 0.70              |
| 34:BM:70:ASP:H    | 34:BM:71:LYS:NZ    | 1.90                     | 0.70              |
| 35:BN:24:MET:HE3  | 35:BN:44:LEU:HD22  | 1.72                     | 0.70              |
| 46:BZ:15:SER:HB2  | 46:BZ:25:ARG:NH1   | 2.06                     | 0.70              |
| 23:DB:98:G:H3'    | 23:DB:99:U:H5''    | 1.71                     | 0.70              |
| 23:DB:1190:G:OP1  | 33:DL:39:LYS:N     | 2.24                     | 0.70              |
| 23:DB:2537:U:H2'  | 23:DB:2538:C:C6    | 2.26                     | 0.70              |
| 25:DC:28:PRO:HG2  | 25:DC:79:ARG:NE    | 2.06                     | 0.70              |
| 26:DD:108:ASP:HB2 | 26:DD:204:LYS:HB2  | 1.74                     | 0.70              |
| 27:DE:143:LEU:N   | 27:DE:143:LEU:HD22 | 2.06                     | 0.70              |
| 28:DF:102:LEU:O   | 28:DF:107:VAL:HB   | 1.91                     | 0.70              |
| 37:DP:76:HIS:CD2  | 37:DP:76:HIS:N     | 2.60                     | 0.70              |
| 42:DU:71:ILE:HD12 | 42:DU:102:ILE:HD12 | 1.74                     | 0.70              |
| 2:AC:5:HIS:HD2    | 2:AC:8:GLY:H       | 1.39                     | 0.70              |
| 16:AQ:76:ARG:NE   | 16:AQ:78:VAL:HG22  | 2.04                     | 0.70              |
| 23:BB:85:G:C5'    | 42:BU:28:LEU:HA    | 2.17                     | 0.70              |
| 23:BB:191:A:H2'   | 23:BB:192:C:C6     | 2.26                     | 0.70              |
| 23:BB:990:A:H1'   | 23:BB:1156:A:C2    | 2.26                     | 0.70              |
| 23:BB:1594:U:H2'  | 23:BB:1595:C:C6    | 2.26                     | 0.70              |
| 24:BV:80:HIS:HD2  | 24:BV:83:LYS:H     | 1.39                     | 0.70              |
| 40:BS:18:ARG:HH12 | 40:BS:25:ARG:HH22  | 1.38                     | 0.70              |
| 41:BT:62:VAL:O    | 41:BT:63:VAL:HG12  | 1.90                     | 0.70              |
| 50:B3:29:ARG:HA   | 50:B3:33:THR:CG2   | 2.22                     | 0.70              |
| 1:CA:545:C:O2'    | 1:CA:546:A:H5'     | 1.90                     | 0.70              |
| 1:CA:865:A:H5'    | 1:CA:1078:U:O4     | 1.92                     | 0.70              |
| 10:CK:28:ASN:HD21 | 10:CK:47:GLY:H     | 1.39                     | 0.70              |
| 21:CU:36:PHE:HB2  | 21:CU:39:LYS:HB2   | 1.74                     | 0.70              |
| 22:DA:61:G:H2'    | 22:DA:62:C:H6      | 1.55                     | 0.70              |
| 23:DB:1794:A:H2'  | 23:DB:1795:C:H6    | 1.57                     | 0.70              |
| 25:DC:29:PHE:HD1  | 25:DC:29:PHE:O     | 1.73                     | 0.70              |
| 37:DP:23:ASP:HA   | 37:DP:49:ILE:HG22  | 1.73                     | 0.70              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:D0:10:SER:O     | 47:D0:14:MET:HB2   | 1.91                     | 0.70              |
| 3:AD:104:MET:HE2   | 3:AD:170:LEU:HD13  | 1.71                     | 0.70              |
| 13:AN:74:ARG:O     | 13:AN:74:ARG:HD3   | 1.90                     | 0.70              |
| 23:BB:1826:G:OP2   | 25:BC:221:GLY:HA2  | 1.90                     | 0.70              |
| 23:BB:2216:G:H2'   | 23:BB:2217:G:C8    | 2.26                     | 0.70              |
| 25:BC:172:THR:HG22 | 25:BC:173:LEU:H    | 1.54                     | 0.70              |
| 29:BG:28:LYS:HD3   | 29:BG:79:THR:HA    | 1.72                     | 0.70              |
| 3:CD:94:GLU:HG2    | 3:CD:185:PRO:HG3   | 1.73                     | 0.70              |
| 9:CJ:11:LYS:HB2    | 9:CJ:97:ASP:HB3    | 1.74                     | 0.70              |
| 10:CK:16:SER:CA    | 10:CK:78:ILE:HA    | 2.20                     | 0.70              |
| 23:DB:596:U:H2'    | 23:DB:597:G:C8     | 2.26                     | 0.70              |
| 30:DH:50:ARG:HG3   | 30:DH:51:ARG:N     | 2.06                     | 0.70              |
| 31:DJ:60:ASP:HB3   | 31:DJ:126:ALA:HB1  | 1.73                     | 0.70              |
| 14:AO:88:ARG:HG3   | 23:BB:716:A:OP1    | 1.91                     | 0.70              |
| 23:BB:181:A:H2'    | 23:BB:182:A:H8     | 1.56                     | 0.70              |
| 23:BB:1015:U:H2'   | 23:BB:1016:G:H8    | 1.57                     | 0.70              |
| 24:BV:80:HIS:HD2   | 24:BV:82:TYR:H     | 1.37                     | 0.70              |
| 27:BE:106:LYS:NZ   | 27:BE:106:LYS:HB2  | 2.07                     | 0.70              |
| 39:BR:18:GLN:HB3   | 39:BR:99:THR:HA    | 1.73                     | 0.70              |
| 43:BW:17:ALA:HA    | 43:BW:35:ILE:O     | 1.92                     | 0.70              |
| 1:CA:17:U:H2'      | 1:CA:18:C:H6       | 1.56                     | 0.70              |
| 23:DB:570:G:H2'    | 23:DB:2030:A:N7    | 2.05                     | 0.70              |
| 23:DB:1099:G:H4'   | 52:DI:4:VAL:HB     | 1.73                     | 0.70              |
| 23:DB:1178:C:H2'   | 23:DB:1179:G:C8    | 2.27                     | 0.70              |
| 23:DB:2246:G:H2'   | 23:DB:2247:A:C8    | 2.27                     | 0.70              |
| 23:DB:2684:U:OP1   | 37:DP:59:THR:HB    | 1.91                     | 0.70              |
| 25:DC:141:HIS:CB   | 25:DC:190:THR:HB   | 2.22                     | 0.70              |
| 26:DD:95:SER:C     | 26:DD:96:ILE:HG13  | 2.16                     | 0.70              |
| 35:DN:2:ARG:HH11   | 35:DN:2:ARG:HG2    | 1.57                     | 0.70              |
| 36:DO:35:ILE:HG12  | 36:DO:106:LEU:HD12 | 1.74                     | 0.70              |
| 36:DO:38:GLN:HA    | 36:DO:50:ALA:HB3   | 1.72                     | 0.70              |
| 47:D0:26:SER:HB2   | 47:D0:38:LEU:HD21  | 1.74                     | 0.70              |
| 1:AA:1219:A:H2'    | 1:AA:1220:G:C8     | 2.27                     | 0.70              |
| 1:AA:1238:A:H5'    | 1:AA:1336:C:H41    | 1.55                     | 0.70              |
| 23:BB:929:U:H5'    | 45:BY:37:ARG:NH1   | 2.07                     | 0.70              |
| 25:BC:180:MET:HE2  | 25:BC:265:PHE:CD2  | 2.27                     | 0.70              |
| 30:BH:17:ASP:OD2   | 30:BH:21:VAL:HB    | 1.92                     | 0.70              |
| 34:BM:3:GLN:CD     | 34:BM:5:LYS:H      | 1.98                     | 0.70              |
| 38:BQ:92:LYS:CG    | 38:BQ:93:ILE:N     | 2.54                     | 0.70              |
| 38:BQ:92:LYS:HA    | 38:BQ:95:ALA:HB2   | 1.72                     | 0.70              |
| 5:CF:38:ARG:HD3    | 5:CF:97:THR:HA     | 1.73                     | 0.70              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DB:2597:G:H5'' | 25:DC:239:PHE:HB2 | 1.74                     | 0.70              |
| 25:DC:144:GLU:HB2 | 25:DC:187:CYS:HB2 | 1.73                     | 0.70              |
| 30:DH:8:LYS:HE2   | 30:DH:9:VAL:H     | 1.56                     | 0.70              |
| 39:DR:70:GLU:HG3  | 39:DR:71:LYS:HG2  | 1.73                     | 0.70              |
| 46:DZ:5:ILE:HG13  | 46:DZ:51:VAL:HG13 | 1.73                     | 0.70              |
| 48:D1:47:ILE:HG22 | 48:D1:48:TYR:N    | 2.03                     | 0.70              |
| 1:AA:1289:A:H2'   | 1:AA:1290:G:H5'   | 1.74                     | 0.70              |
| 8:AI:40:ARG:N     | 8:AI:44:ARG:HE    | 1.88                     | 0.70              |
| 17:AR:58:ILE:O    | 17:AR:62:ARG:HG3  | 1.92                     | 0.70              |
| 22:BA:98:G:H1     | 24:BV:14:LYS:HB2  | 1.55                     | 0.70              |
| 23:BB:1794:A:H2'  | 23:BB:1795:C:C6   | 2.26                     | 0.70              |
| 23:BB:1794:A:H2'  | 23:BB:1795:C:H6   | 1.57                     | 0.70              |
| 23:BB:2297:A:H61  | 23:BB:2319:G:H3'  | 1.54                     | 0.70              |
| 23:BB:2834:G:H1'  | 23:BB:2883:A:N6   | 2.06                     | 0.70              |
| 34:BM:23:GLY:N    | 34:BM:96:ILE:HD12 | 2.06                     | 0.70              |
| 46:BZ:69:SER:O    | 46:BZ:70:LYS:HB2  | 1.91                     | 0.70              |
| 1:CA:188:C:H2'    | 1:CA:189:A:O4'    | 1.90                     | 0.70              |
| 1:CA:960:U:O2'    | 1:CA:961:U:OP2    | 2.09                     | 0.70              |
| 1:CA:1007:U:H2'   | 1:CA:1008:U:C6    | 2.27                     | 0.70              |
| 1:CA:1216:A:OP1   | 13:CN:2:LYS:HE2   | 1.91                     | 0.70              |
| 1:CA:1342:C:H5'   | 8:CI:127:SER:HB3  | 1.72                     | 0.70              |
| 1:CA:1391:U:H2'   | 1:CA:1392:G:C8    | 2.26                     | 0.70              |
| 18:CS:48:ILE:O    | 18:CS:59:VAL:HG22 | 1.90                     | 0.70              |
| 23:DB:1113:U:H5'  | 29:DG:2:ARG:HG2   | 1.72                     | 0.70              |
| 23:DB:1794:A:H2'  | 23:DB:1795:C:C6   | 2.26                     | 0.70              |
| 39:DR:96:VAL:HG12 | 39:DR:98:ILE:HG12 | 1.72                     | 0.70              |
| 41:DT:17:SER:H    | 41:DT:20:ALA:HB3  | 1.55                     | 0.70              |
| 1:AA:1071:C:H2'   | 1:AA:1072:G:H8    | 1.55                     | 0.70              |
| 3:AD:2:ARG:NH1    | 3:AD:114:ARG:HD2  | 2.05                     | 0.70              |
| 3:AD:25:ARG:HD3   | 3:AD:26:ALA:H     | 1.56                     | 0.70              |
| 23:BB:2557:G:H2'  | 23:BB:2558:C:C6   | 2.27                     | 0.70              |
| 24:BV:40:ILE:HD13 | 24:BV:40:ILE:H    | 1.56                     | 0.70              |
| 42:BU:25:LYS:HG2  | 42:BU:35:VAL:HG22 | 1.74                     | 0.70              |
| 43:BW:36:ILE:HB   | 43:BW:68:PHE:HD2  | 1.57                     | 0.70              |
| 1:CA:939:G:H5''   | 6:CG:101:ARG:NH1  | 2.06                     | 0.70              |
| 23:DB:28:A:H61    | 23:DB:512:G:H1'   | 1.57                     | 0.70              |
| 23:DB:969:G:H2'   | 23:DB:970:U:C6    | 2.26                     | 0.70              |
| 23:DB:1064:C:C4'  | 52:DI:90:GLY:HA2  | 2.21                     | 0.70              |
| 23:DB:1485:U:H2'  | 23:DB:1486:U:C6   | 2.26                     | 0.70              |
| 31:DJ:84:ILE:CD1  | 31:DJ:85:LYS:H    | 2.04                     | 0.70              |
| 32:DK:110:GLU:HA  | 32:DK:113:MET:HG2 | 1.74                     | 0.70              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:DT:68:LYS:NZ   | 41:DT:68:LYS:HB2  | 2.07                     | 0.70              |
| 14:AO:11:VAL:HG23 | 14:AO:26:VAL:HG11 | 1.72                     | 0.69              |
| 16:AQ:10:ARG:HH11 | 16:AQ:55:GLY:H    | 1.37                     | 0.69              |
| 23:BB:150:U:H2'   | 23:BB:151:C:C6    | 2.27                     | 0.69              |
| 23:BB:1188:U:H4'  | 39:BR:83:TYR:HB2  | 1.74                     | 0.69              |
| 23:BB:2270:A:H4'  | 43:BW:18:LYS:CG   | 2.21                     | 0.69              |
| 26:BD:119:ALA:HA  | 26:BD:123:LYS:NZ  | 2.06                     | 0.69              |
| 20:CB:8:MET:SD    | 20:CB:9:LEU:HD22  | 2.32                     | 0.69              |
| 23:DB:336:C:H5''  | 42:DU:3:LYS:NZ    | 2.06                     | 0.69              |
| 23:DB:1346:G:O2'  | 23:DB:1347:A:H5'  | 1.92                     | 0.69              |
| 25:DC:63:ILE:HG21 | 25:DC:90:ILE:CD1  | 2.22                     | 0.69              |
| 44:DX:42:LEU:C    | 44:DX:43:LEU:HD22 | 2.17                     | 0.69              |
| 1:AA:1236:A:H4'   | 1:AA:1304:G:H4'   | 1.73                     | 0.69              |
| 14:AO:87:ARG:HA   | 14:AO:87:ARG:NH1  | 2.07                     | 0.69              |
| 23:BB:2619:C:H5'  | 26:BD:157:LYS:CE  | 2.21                     | 0.69              |
| 35:BN:4:ARG:HD2   | 35:BN:5:LYS:H     | 1.56                     | 0.69              |
| 35:BN:33:ILE:HD13 | 35:BN:33:ILE:H    | 1.56                     | 0.69              |
| 37:BP:32:VAL:HG13 | 37:BP:40:GLN:HE21 | 1.57                     | 0.69              |
| 43:BW:10:ARG:HH11 | 43:BW:10:ARG:HB3  | 1.57                     | 0.69              |
| 1:CA:279:A:H5''   | 1:CA:280:C:H3'    | 1.72                     | 0.69              |
| 7:CH:55:LYS:HA    | 7:CH:55:LYS:NZ    | 2.07                     | 0.69              |
| 16:CQ:19:SER:O    | 16:CQ:20:ILE:HD12 | 1.93                     | 0.69              |
| 23:DB:172:A:H2'   | 23:DB:173:A:C8    | 2.27                     | 0.69              |
| 23:DB:522:A:H2'   | 23:DB:523:C:C6    | 2.27                     | 0.69              |
| 23:DB:920:A:H2'   | 23:DB:921:C:C6    | 2.27                     | 0.69              |
| 23:DB:2147:A:H4'  | 23:DB:2148:G:H8   | 1.57                     | 0.69              |
| 23:DB:2636:C:H5'  | 26:DD:80:TRP:HZ2  | 1.57                     | 0.69              |
| 29:DG:155:PRO:CB  | 29:DG:171:LYS:HB3 | 2.21                     | 0.69              |
| 37:DP:31:VAL:HG13 | 37:DP:81:ASP:HB3  | 1.73                     | 0.69              |
| 40:DS:73:LYS:HD3  | 40:DS:74:ILE:N    | 2.06                     | 0.69              |
| 46:DZ:47:LYS:HB2  | 46:DZ:51:VAL:HG12 | 1.74                     | 0.69              |
| 1:AA:473:U:H2'    | 1:AA:474:G:H8     | 1.58                     | 0.69              |
| 23:BB:38:A:H2'    | 23:BB:39:G:O4'    | 1.92                     | 0.69              |
| 23:BB:150:U:H2'   | 23:BB:151:C:H6    | 1.56                     | 0.69              |
| 23:BB:1373:A:H2'  | 23:BB:1374:G:O4'  | 1.92                     | 0.69              |
| 23:BB:1406:U:H2'  | 23:BB:1407:G:C8   | 2.27                     | 0.69              |
| 26:BD:11:MET:SD   | 37:BP:9:GLN:HG2   | 2.32                     | 0.69              |
| 27:BE:146:VAL:O   | 27:BE:184:ASP:HB2 | 1.92                     | 0.69              |
| 34:BM:133:LYS:HE3 | 34:BM:133:LYS:O   | 1.93                     | 0.69              |
| 1:CA:1320:C:N3    | 18:CS:35:ARG:HD3  | 2.06                     | 0.69              |
| 2:CC:39:ARG:HH22  | 13:CN:91:GLU:HB3  | 1.58                     | 0.69              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:CH:55:LYS:HA    | 7:CH:55:LYS:HZ2    | 1.56                     | 0.69              |
| 23:DB:151:C:H2'   | 23:DB:152:A:C8     | 2.27                     | 0.69              |
| 23:DB:1098:A:H2'  | 52:DI:4:VAL:CA     | 2.22                     | 0.69              |
| 28:DF:162:ASP:O   | 28:DF:166:ARG:HG3  | 1.92                     | 0.69              |
| 31:DJ:114:LEU:HG  | 31:DJ:118:MET:HE1  | 1.73                     | 0.69              |
| 51:D4:1:MET:HB3   | 51:D4:2:LYS:HD3    | 1.74                     | 0.69              |
| 1:AA:413:G:O6     | 3:AD:32:LYS:HE3    | 1.93                     | 0.69              |
| 20:AB:59:ILE:HD12 | 20:AB:60:ALA:N     | 2.07                     | 0.69              |
| 21:AU:36:PHE:HB3  | 21:AU:40:PRO:CD    | 2.21                     | 0.69              |
| 25:BC:164:VAL:HB  | 25:BC:167:ASP:OD1  | 1.92                     | 0.69              |
| 31:BJ:68:LYS:HA   | 31:BJ:71:ASP:OD1   | 1.93                     | 0.69              |
| 36:BO:41:ALA:HB1  | 36:BO:42:PRO:HD2   | 1.74                     | 0.69              |
| 37:BP:2:ASN:HD22  | 37:BP:2:ASN:N      | 1.89                     | 0.69              |
| 37:BP:18:SER:HA   | 37:BP:87:ARG:NH2   | 2.07                     | 0.69              |
| 40:BS:7:HIS:HB2   | 40:BS:103:ILE:HG22 | 1.72                     | 0.69              |
| 41:BT:64:LYS:HD2  | 41:BT:77:ARG:HD3   | 1.75                     | 0.69              |
| 42:BU:46:LYS:N    | 42:BU:47:PRO:HD3   | 2.08                     | 0.69              |
| 51:B4:24:ARG:HA   | 51:B4:34:LYS:O     | 1.93                     | 0.69              |
| 1:CA:1508:A:H2'   | 1:CA:1509:C:H6     | 1.56                     | 0.69              |
| 12:CM:92:ARG:CZ   | 12:CM:92:ARG:HA    | 2.22                     | 0.69              |
| 23:DB:2578:G:O2'  | 26:DD:138:LEU:HD13 | 1.93                     | 0.69              |
| 23:DB:2636:C:H5'  | 26:DD:80:TRP:CZ2   | 2.28                     | 0.69              |
| 23:DB:2834:G:H1'  | 23:DB:2883:A:N6    | 2.06                     | 0.69              |
| 24:DV:21:ARG:HE   | 24:DV:87:GLN:HA    | 1.57                     | 0.69              |
| 26:DD:30:GLU:HG2  | 26:DD:94:GLN:NE2   | 2.07                     | 0.69              |
| 27:DE:83:VAL:O    | 27:DE:84:THR:HG22  | 1.92                     | 0.69              |
| 41:DT:66:LYS:N    | 41:DT:76:ARG:HH21  | 1.87                     | 0.69              |
| 1:AA:1432:G:OP1   | 37:BP:105:LYS:HB2  | 1.93                     | 0.69              |
| 22:BA:6:G:H2'     | 22:BA:7:G:C8       | 2.27                     | 0.69              |
| 23:BB:45:G:C5'    | 23:BB:46:G:H5'     | 2.22                     | 0.69              |
| 23:BB:1132:U:H5'' | 31:BJ:85:LYS:HZ3   | 1.57                     | 0.69              |
| 23:BB:2469:A:H4'  | 34:BM:55:ARG:HG3   | 1.75                     | 0.69              |
| 24:BV:77:VAL:HA   | 24:BV:89:ILE:HG22  | 1.74                     | 0.69              |
| 37:BP:77:SER:H    | 37:BP:78:PRO:CD    | 2.06                     | 0.69              |
| 11:CL:51:VAL:HG12 | 11:CL:52:CYS:H     | 1.57                     | 0.69              |
| 25:DC:53:ILE:HG12 | 25:DC:218:THR:HA   | 1.74                     | 0.69              |
| 25:DC:179:GLU:CD  | 25:DC:266:ILE:HA   | 2.17                     | 0.69              |
| 27:DE:136:GLN:O   | 27:DE:139:LYS:HG2  | 1.93                     | 0.69              |
| 27:DE:163:ASN:H   | 27:DE:168:ASP:HA   | 1.58                     | 0.69              |
| 41:DT:56:GLU:HG2  | 41:DT:57:VAL:HG13  | 1.75                     | 0.69              |
| 48:D1:45:HIS:O    | 48:D1:46:VAL:HG12  | 1.92                     | 0.69              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:60:A:H4'     | 1:AA:61:G:O5'      | 1.92                     | 0.69              |
| 1:AA:270:A:H2'    | 1:AA:271:C:H6      | 1.57                     | 0.69              |
| 1:AA:1048:G:H4'   | 13:AN:2:LYS:NZ     | 2.07                     | 0.69              |
| 5:AF:86:ARG:HH11  | 17:AR:63:TYR:HB3   | 1.57                     | 0.69              |
| 15:AP:5:ARG:H     | 15:AP:5:ARG:HD2    | 1.57                     | 0.69              |
| 16:AQ:11:VAL:HA   | 16:AQ:22:VAL:HG22  | 1.73                     | 0.69              |
| 20:AB:76:SER:O    | 20:AB:79:VAL:HG12  | 1.93                     | 0.69              |
| 23:BB:596:U:H2'   | 23:BB:597:G:C8     | 2.27                     | 0.69              |
| 23:BB:2037:A:H2'  | 23:BB:2038:G:H8    | 1.58                     | 0.69              |
| 23:BB:2241:A:H2'  | 23:BB:2242:G:H8    | 1.57                     | 0.69              |
| 23:BB:2645:G:H3'  | 23:BB:2646:C:C5'   | 2.23                     | 0.69              |
| 23:BB:2804:U:H2'  | 23:BB:2805:C:C6    | 2.28                     | 0.69              |
| 25:BC:170:TYR:O   | 25:BC:171:VAL:HG13 | 1.91                     | 0.69              |
| 27:BE:98:LYS:HG3  | 27:BE:99:LYS:H     | 1.56                     | 0.69              |
| 31:BJ:6:ALA:O     | 31:BJ:8:PRO:HD3    | 1.93                     | 0.69              |
| 32:BK:85:VAL:HG11 | 32:BK:115:ILE:HD12 | 1.74                     | 0.69              |
| 34:BM:69:PRO:HB2  | 34:BM:71:LYS:NZ    | 2.08                     | 0.69              |
| 38:BQ:96:ASP:O    | 38:BQ:99:VAL:HG22  | 1.92                     | 0.69              |
| 38:BQ:102:LYS:HD2 | 38:BQ:102:LYS:H    | 1.58                     | 0.69              |
| 39:BR:79:ARG:HD3  | 39:BR:86:GLN:NE2   | 2.08                     | 0.69              |
| 42:BU:23:LYS:HZ3  | 42:BU:24:VAL:HG22  | 1.58                     | 0.69              |
| 47:B0:30:ASP:OD1  | 47:B0:31:LYS:HD2   | 1.93                     | 0.69              |
| 50:B3:26:ALA:HB1  | 50:B3:29:ARG:HG2   | 1.73                     | 0.69              |
| 1:CA:832:G:O2'    | 1:CA:833:G:H5'     | 1.92                     | 0.69              |
| 1:CA:1250:A:H2'   | 1:CA:1251:A:C8     | 2.28                     | 0.69              |
| 10:CK:85:VAL:HG21 | 10:CK:92:ARG:HH12  | 1.58                     | 0.69              |
| 23:DB:1309:G:H5'  | 49:D2:8:SER:H      | 1.58                     | 0.69              |
| 23:DB:1552:A:H2'  | 23:DB:1553:A:H5'   | 1.73                     | 0.69              |
| 23:DB:2017:U:O2   | 47:D0:6:LYS:HG3    | 1.92                     | 0.69              |
| 1:AA:978:A:H5'    | 1:AA:1362:A:N6     | 2.08                     | 0.69              |
| 1:AA:1218:C:H2'   | 1:AA:1219:A:C8     | 2.28                     | 0.69              |
| 25:BC:141:HIS:CD2 | 25:BC:193:GLU:H    | 2.11                     | 0.69              |
| 43:BW:66:VAL:HG13 | 43:BW:67:LYS:N     | 2.04                     | 0.69              |
| 51:B4:24:ARG:HH22 | 51:B4:36:ARG:CD    | 2.03                     | 0.69              |
| 2:CC:11:LEU:HD22  | 2:CC:17:TRP:HE1    | 1.58                     | 0.69              |
| 8:CI:118:ARG:NH2  | 8:CI:122:ARG:HE    | 1.90                     | 0.69              |
| 22:DA:66:A:O2'    | 22:DA:67:G:H5''    | 1.93                     | 0.69              |
| 23:DB:1118:C:H2'  | 23:DB:1119:U:C6    | 2.27                     | 0.69              |
| 23:DB:1866:A:H2'  | 23:DB:1867:G:O4'   | 1.93                     | 0.69              |
| 23:DB:2229:U:H2'  | 23:DB:2230:G:C8    | 2.27                     | 0.69              |
| 23:DB:2645:G:H3'  | 23:DB:2646:C:C5'   | 2.22                     | 0.69              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DE:15:SER:HB3   | 27:DE:196:VAL:HG22 | 1.74                     | 0.69              |
| 27:DE:46:GLN:NE2   | 27:DE:86:ALA:HB3   | 2.07                     | 0.69              |
| 30:DH:5:LEU:HD13   | 30:DH:35:LYS:HE3   | 1.74                     | 0.69              |
| 31:DJ:131:ASN:C    | 31:DJ:133:ALA:H    | 2.01                     | 0.69              |
| 31:DJ:135:GLN:HE21 | 31:DJ:138:GLN:H    | 1.40                     | 0.69              |
| 36:DO:15:ARG:HH12  | 43:DW:76:ARG:NE    | 1.91                     | 0.69              |
| 1:AA:451:A:H4'     | 1:AA:452:A:O4'     | 1.91                     | 0.69              |
| 1:AA:1060:U:H2'    | 1:AA:1061:G:H8     | 1.58                     | 0.69              |
| 8:AI:18:VAL:HG11   | 8:AI:82:ILE:HG12   | 1.75                     | 0.69              |
| 20:AB:53:LEU:HA    | 20:AB:56:LEU:HD22  | 1.74                     | 0.69              |
| 23:BB:215:G:H4'    | 23:BB:216:A:H4'    | 1.75                     | 0.69              |
| 23:BB:437:U:H2'    | 23:BB:438:G:C8     | 2.27                     | 0.69              |
| 23:BB:1243:C:O2'   | 33:BL:15:ALA:HB3   | 1.92                     | 0.69              |
| 23:BB:1252:G:H1    | 38:BQ:36:GLN:HE22  | 1.39                     | 0.69              |
| 23:BB:1799:G:H4'   | 23:BB:1800:C:O5'   | 1.93                     | 0.69              |
| 23:BB:2355:G:H4'   | 43:BW:20:LEU:HD22  | 1.75                     | 0.69              |
| 25:BC:79:ARG:HH11  | 25:BC:80:LEU:H     | 1.38                     | 0.69              |
| 25:BC:127:ASN:HD22 | 25:BC:128:THR:N    | 1.91                     | 0.69              |
| 30:BH:82:SER:N     | 30:BH:146:VAL:HG13 | 2.00                     | 0.69              |
| 31:BJ:28:LEU:HD23  | 31:BJ:29:ALA:N     | 2.08                     | 0.69              |
| 1:CA:412:A:H1'     | 1:CA:413:G:H8      | 1.57                     | 0.69              |
| 1:CA:473:U:H2'     | 1:CA:474:G:H8      | 1.58                     | 0.69              |
| 1:CA:1096:C:H2'    | 1:CA:1097:C:C6     | 2.28                     | 0.69              |
| 1:CA:1281:C:H5'    | 1:CA:1282:C:H5     | 1.56                     | 0.69              |
| 9:CJ:39:PRO:HA     | 9:CJ:74:VAL:HG22   | 1.74                     | 0.69              |
| 22:DA:22:U:H2'     | 22:DA:23:G:C8      | 2.28                     | 0.69              |
| 23:DB:682:G:H5'    | 49:D2:26:ASN:ND2   | 2.08                     | 0.69              |
| 23:DB:993:G:H21    | 39:DR:93:PHE:HZ    | 1.41                     | 0.69              |
| 23:DB:1098:A:OP2   | 52:DI:3:LYS:HG2    | 1.92                     | 0.69              |
| 23:DB:2834:G:H1'   | 23:DB:2883:A:H61   | 1.58                     | 0.69              |
| 27:DE:108:ILE:HG13 | 27:DE:109:LEU:H    | 1.58                     | 0.69              |
| 31:DJ:124:VAL:HG23 | 31:DJ:125:TYR:N    | 2.07                     | 0.69              |
| 32:DK:64:ARG:HD2   | 32:DK:102:PRO:O    | 1.91                     | 0.69              |
| 34:DM:42:THR:HG1   | 34:DM:91:TYR:HD2   | 1.41                     | 0.69              |
| 39:DR:3:ALA:O      | 39:DR:4:VAL:HG13   | 1.93                     | 0.69              |
| 39:DR:22:LEU:HD12  | 39:DR:23:GLU:H     | 1.57                     | 0.69              |
| 39:DR:49:ILE:HG13  | 39:DR:51:VAL:HG23  | 1.74                     | 0.69              |
| 42:DU:91:LYS:HD3   | 42:DU:93:ARG:NE    | 2.07                     | 0.69              |
| 45:DY:7:THR:HA     | 45:DY:34:THR:HB    | 1.75                     | 0.69              |
| 46:DZ:25:ARG:HG3   | 46:DZ:26:SER:H     | 1.58                     | 0.69              |
| 48:D1:29:LYS:HB2   | 48:D1:30:PRO:CD    | 2.18                     | 0.69              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:131:A:H2'    | 1:AA:132:C:C6      | 2.28                     | 0.69              |
| 1:AA:832:G:O2'    | 1:AA:833:G:H5'     | 1.92                     | 0.69              |
| 1:AA:1524:C:H2'   | 1:AA:1525:G:C8     | 2.28                     | 0.69              |
| 2:AC:9:ILE:HG23   | 2:AC:10:ARG:HG3    | 1.73                     | 0.69              |
| 5:AF:3:HIS:HA     | 5:AF:65:GLU:HA     | 1.75                     | 0.69              |
| 7:AH:87:ARG:HB2   | 7:AH:90:GLU:HG3    | 1.74                     | 0.69              |
| 10:AK:109:ILE:H   | 21:AU:5:VAL:HB     | 1.57                     | 0.69              |
| 23:BB:743:A:O2'   | 23:BB:744:U:H5'    | 1.93                     | 0.69              |
| 23:BB:1866:A:H2'  | 23:BB:1867:G:O4'   | 1.93                     | 0.69              |
| 29:BG:97:VAL:HG11 | 29:BG:122:ALA:O    | 1.92                     | 0.69              |
| 34:BM:100:LYS:O   | 34:BM:100:LYS:HD2  | 1.93                     | 0.69              |
| 47:B0:26:SER:HB2  | 47:B0:38:LEU:HD12  | 1.74                     | 0.69              |
| 47:B0:29:VAL:HG21 | 47:B0:41:HIS:ND1   | 2.08                     | 0.69              |
| 23:DB:1099:G:O5'  | 52:DI:4:VAL:HG12   | 1.92                     | 0.69              |
| 27:DE:115:GLN:HG3 | 27:DE:116:ASP:H    | 1.58                     | 0.69              |
| 29:DG:95:ALA:HB1  | 29:DG:130:ILE:HD11 | 1.73                     | 0.69              |
| 33:DL:64:PHE:HA   | 50:D3:11:LYS:HA    | 1.75                     | 0.69              |
| 34:DM:5:LYS:HG3   | 34:DM:69:PRO:O     | 1.93                     | 0.69              |
| 36:DO:7:ARG:O     | 36:DO:11:ALA:HB2   | 1.93                     | 0.69              |
| 40:DS:48:LYS:O    | 40:DS:52:GLU:HG3   | 1.92                     | 0.69              |
| 46:DZ:3:LYS:HG3   | 46:DZ:48:GLN:H     | 1.58                     | 0.69              |
| 49:D2:21:ARG:HG3  | 49:D2:31:LEU:HD11  | 1.75                     | 0.69              |
| 52:DI:85:ILE:HD13 | 52:DI:137:LEU:HD21 | 1.75                     | 0.69              |
| 8:AI:12:LYS:H     | 8:AI:109:GLN:HE22  | 1.41                     | 0.69              |
| 23:BB:845:A:C2    | 23:BB:847:U:H1'    | 2.27                     | 0.69              |
| 23:BB:2265:U:H3'  | 23:BB:2266:A:H5''  | 1.75                     | 0.69              |
| 25:BC:68:ARG:HD2  | 25:BC:127:ASN:HD21 | 1.57                     | 0.69              |
| 42:BU:54:PRO:HG2  | 42:BU:55:GLY:H     | 1.58                     | 0.69              |
| 50:B3:31:ILE:HG22 | 50:B3:32:LEU:HG    | 1.75                     | 0.69              |
| 1:CA:131:A:H2'    | 1:CA:132:C:C6      | 2.28                     | 0.69              |
| 1:CA:1218:C:H2'   | 1:CA:1219:A:H8     | 1.56                     | 0.69              |
| 23:DB:1440:U:H2'  | 23:DB:1441:G:C8    | 2.28                     | 0.69              |
| 23:DB:2229:U:H2'  | 23:DB:2230:G:H8    | 1.56                     | 0.69              |
| 34:DM:64:TRP:HB2  | 34:DM:102:LEU:HB2  | 1.75                     | 0.69              |
| 40:DS:83:LYS:HD3  | 40:DS:83:LYS:N     | 2.07                     | 0.69              |
| 1:AA:412:A:H1'    | 1:AA:413:G:H8      | 1.57                     | 0.68              |
| 1:AA:673:A:H2'    | 1:AA:674:G:C8      | 2.29                     | 0.68              |
| 1:AA:865:A:H5'    | 1:AA:1078:U:O4     | 1.93                     | 0.68              |
| 1:AA:1330:U:C2'   | 1:AA:1331:G:H5'    | 2.22                     | 0.68              |
| 3:AD:60:VAL:HA    | 3:AD:63:ILE:HD12   | 1.74                     | 0.68              |
| 23:BB:1060:U:O2   | 23:BB:1088:A:N7    | 2.27                     | 0.68              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:1791:A:H1'   | 25:BC:206:LYS:NZ   | 2.08                     | 0.68              |
| 23:BB:2849:U:H4'   | 23:BB:2850:A:H5'   | 1.74                     | 0.68              |
| 33:BL:118:THR:CB   | 33:BL:119:PRO:HD3  | 2.22                     | 0.68              |
| 36:BO:68:LYS:HD3   | 36:BO:68:LYS:H     | 1.58                     | 0.68              |
| 40:BS:7:HIS:CD2    | 40:BS:8:ARG:H      | 2.11                     | 0.68              |
| 1:CA:270:A:H2'     | 1:CA:271:C:H6      | 1.57                     | 0.68              |
| 1:CA:642:A:H2'     | 1:CA:643:C:H6      | 1.58                     | 0.68              |
| 5:CF:47:LEU:HD12   | 5:CF:55:HIS:HA     | 1.75                     | 0.68              |
| 23:DB:532:A:N1     | 23:DB:2020:A:H1'   | 2.08                     | 0.68              |
| 33:DL:35:HIS:NE2   | 39:DR:84:ARG:HG2   | 2.08                     | 0.68              |
| 39:DR:37:GLU:HG3   | 39:DR:62:GLU:HG3   | 1.74                     | 0.68              |
| 48:D1:10:LEU:H     | 48:D1:24:LYS:HB3   | 1.58                     | 0.68              |
| 4:AE:155:LYS:HE3   | 7:AH:70:VAL:HG13   | 1.75                     | 0.68              |
| 9:AJ:50:THR:HG22   | 9:AJ:64:GLN:HG2    | 1.75                     | 0.68              |
| 23:BB:181:A:H2'    | 23:BB:182:A:C8     | 2.28                     | 0.68              |
| 23:BB:423:A:H5'    | 23:BB:424:G:H5''   | 1.75                     | 0.68              |
| 23:BB:1346:G:O2'   | 23:BB:1347:A:H5'   | 1.92                     | 0.68              |
| 23:BB:1552:A:H2'   | 23:BB:1553:A:H5'   | 1.74                     | 0.68              |
| 25:BC:72:GLY:C     | 25:BC:73:ILE:HD12  | 2.18                     | 0.68              |
| 25:BC:124:LYS:HB2  | 25:BC:125:PRO:HD3  | 1.75                     | 0.68              |
| 29:BG:120:ILE:HG12 | 29:BG:140:ILE:HG22 | 1.74                     | 0.68              |
| 31:BJ:24:THR:C     | 31:BJ:25:LEU:HD22  | 2.17                     | 0.68              |
| 31:BJ:36:LEU:HD11  | 31:BJ:122:LEU:HD23 | 1.75                     | 0.68              |
| 37:BP:59:THR:O     | 37:BP:60:VAL:HG13  | 1.94                     | 0.68              |
| 46:BZ:5:ILE:HB     | 46:BZ:51:VAL:CG1   | 2.23                     | 0.68              |
| 1:CA:98:A:H2'      | 1:CA:99:C:C6       | 2.28                     | 0.68              |
| 1:CA:203:G:H1'     | 1:CA:465:A:H62     | 1.58                     | 0.68              |
| 1:CA:977:A:H3'     | 1:CA:1362:A:H62    | 1.56                     | 0.68              |
| 2:CC:156:LEU:HB2   | 2:CC:163:ARG:HD3   | 1.73                     | 0.68              |
| 8:CI:20:ILE:HG23   | 8:CI:60:LEU:HD13   | 1.74                     | 0.68              |
| 20:CB:83:ALA:O     | 20:CB:88:GLN:HB2   | 1.93                     | 0.68              |
| 21:CU:14:ALA:H     | 21:CU:16:ARG:HH22  | 1.41                     | 0.68              |
| 23:DB:1406:U:H2'   | 23:DB:1407:G:C8    | 2.28                     | 0.68              |
| 23:DB:2054:A:H2'   | 47:D0:4:GLN:NE2    | 2.08                     | 0.68              |
| 32:DK:64:ARG:H     | 32:DK:83:ALA:HB3   | 1.58                     | 0.68              |
| 23:BB:65:U:H4'     | 41:BT:70:HIS:ND1   | 2.09                     | 0.68              |
| 23:BB:974:G:H1'    | 23:BB:975:A:C8     | 2.27                     | 0.68              |
| 23:BB:2071:A:H2'   | 23:BB:2072:C:C6    | 2.28                     | 0.68              |
| 23:BB:2901:C:H2'   | 23:BB:2902:C:H5'   | 1.74                     | 0.68              |
| 25:BC:61:TYR:HD2   | 25:BC:84:PRO:HD2   | 1.58                     | 0.68              |
| 28:BF:46:LYS:O     | 28:BF:50:ASP:HB3   | 1.94                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:BG:176:LYS:HE2  | 29:BG:176:LYS:O    | 1.93                     | 0.68              |
| 31:BJ:93:ILE:HD13  | 31:BJ:100:VAL:HG21 | 1.74                     | 0.68              |
| 1:CA:1328:C:H5''   | 12:CM:27:THR:HG21  | 1.75                     | 0.68              |
| 23:DB:2037:A:H2'   | 23:DB:2038:G:H8    | 1.58                     | 0.68              |
| 23:DB:2246:G:H2'   | 23:DB:2247:A:H8    | 1.58                     | 0.68              |
| 23:DB:2804:U:H2'   | 23:DB:2805:C:C6    | 2.27                     | 0.68              |
| 23:DB:2804:U:H2'   | 23:DB:2805:C:H6    | 1.58                     | 0.68              |
| 23:DB:2860:A:H8    | 23:DB:2860:A:O5'   | 1.76                     | 0.68              |
| 25:DC:89:ASN:HB2   | 25:DC:105:ALA:HB3  | 1.75                     | 0.68              |
| 29:DG:17:LYS:HE2   | 29:DG:24:THR:H     | 1.59                     | 0.68              |
| 43:DW:56:HIS:HA    | 43:DW:77:LYS:HE2   | 1.75                     | 0.68              |
| 46:DZ:39:LYS:HD3   | 46:DZ:61:ASN:ND2   | 2.09                     | 0.68              |
| 20:AB:9:LEU:HD22   | 20:AB:11:ALA:N     | 2.07                     | 0.68              |
| 23:BB:594:U:H2'    | 23:BB:595:C:C6     | 2.28                     | 0.68              |
| 23:BB:720:U:H2'    | 23:BB:721:A:C8     | 2.28                     | 0.68              |
| 23:BB:1803:A:O3'   | 25:BC:254:LYS:HG2  | 1.94                     | 0.68              |
| 23:BB:2795:C:H2'   | 23:BB:2796:U:O4'   | 1.94                     | 0.68              |
| 23:BB:2860:A:H8    | 23:BB:2860:A:O5'   | 1.76                     | 0.68              |
| 33:BL:30:THR:HG22  | 33:BL:36:LYS:NZ    | 2.07                     | 0.68              |
| 42:BU:25:LYS:HA    | 42:BU:35:VAL:H     | 1.58                     | 0.68              |
| 43:BW:43:LYS:HG2   | 43:BW:76:ARG:HE    | 1.57                     | 0.68              |
| 1:CA:1057:G:H4'    | 2:CC:196:GLY:H     | 1.58                     | 0.68              |
| 3:CD:141:VAL:HA    | 3:CD:180:THR:H     | 1.58                     | 0.68              |
| 8:CI:70:GLY:O      | 8:CI:74:GLN:HG2    | 1.93                     | 0.68              |
| 23:DB:947:A:H2'    | 23:DB:948:C:C6     | 2.29                     | 0.68              |
| 23:DB:1082:U:C4    | 23:DB:1086:A:C2    | 2.81                     | 0.68              |
| 26:DD:34:VAL:H     | 26:DD:90:PHE:C     | 2.01                     | 0.68              |
| 26:DD:79:LEU:HG    | 26:DD:80:TRP:H     | 1.57                     | 0.68              |
| 30:DH:1:MET:C      | 30:DH:21:VAL:HG22  | 2.19                     | 0.68              |
| 30:DH:26:ALA:HB3   | 30:DH:31:VAL:HG23  | 1.74                     | 0.68              |
| 51:D4:15:LYS:NZ    | 51:D4:22:VAL:HG12  | 2.06                     | 0.68              |
| 51:D4:26:ILE:HG13  | 51:D4:35:GLN:N     | 2.03                     | 0.68              |
| 1:AA:642:A:H2'     | 1:AA:643:C:H6      | 1.58                     | 0.68              |
| 9:AJ:56:HIS:H      | 13:AN:80:ARG:HH22  | 1.41                     | 0.68              |
| 10:AK:70:ALA:HB1   | 10:AK:74:LYS:HE3   | 1.75                     | 0.68              |
| 10:AK:97:ARG:HB3   | 10:AK:97:ARG:NH1   | 2.08                     | 0.68              |
| 22:BA:17:C:O2'     | 22:BA:18:G:H5'     | 1.93                     | 0.68              |
| 23:BB:139:U:H5''   | 23:BB:140:C:C5     | 2.27                     | 0.68              |
| 23:BB:322:A:OP1    | 27:BE:162:ARG:HG2  | 1.93                     | 0.68              |
| 23:BB:1440:U:H2'   | 23:BB:1441:G:C8    | 2.28                     | 0.68              |
| 27:BE:113:VAL:HG23 | 27:BE:117:ARG:NH2  | 2.09                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BE:156:ASN:ND2 | 27:BE:157:LEU:HG   | 2.09                     | 0.68              |
| 39:BR:39:LEU:O    | 39:BR:54:VAL:CG1   | 2.41                     | 0.68              |
| 44:BX:30:MET:HG3  | 44:BX:31:GLN:H     | 1.58                     | 0.68              |
| 18:CS:10:ILE:HB   | 18:CS:14:LEU:HD11  | 1.75                     | 0.68              |
| 18:CS:51:HIS:HA   | 18:CS:56:HIS:HA    | 1.75                     | 0.68              |
| 23:DB:533:G:H2'   | 23:DB:534:U:C6     | 2.28                     | 0.68              |
| 23:DB:857:G:O2'   | 23:DB:858:G:H5'    | 1.94                     | 0.68              |
| 23:DB:1098:A:C2'  | 52:DI:4:VAL:N      | 2.55                     | 0.68              |
| 25:DC:63:ILE:HD13 | 25:DC:90:ILE:HD13  | 1.76                     | 0.68              |
| 27:DE:161:ALA:O   | 27:DE:169:VAL:HB   | 1.93                     | 0.68              |
| 31:DJ:19:ASP:HB3  | 31:DJ:21:THR:HG23  | 1.75                     | 0.68              |
| 33:DL:124:GLY:H   | 33:DL:142:ILE:CA   | 2.07                     | 0.68              |
| 35:DN:97:ILE:HA   | 35:DN:113:ILE:HD13 | 1.74                     | 0.68              |
| 38:DQ:108:LEU:HA  | 38:DQ:111:LYS:HD2  | 1.76                     | 0.68              |
| 50:D3:32:LEU:CD1  | 50:D3:33:THR:H     | 2.06                     | 0.68              |
| 1:AA:194:C:O2'    | 1:AA:195:A:H5'     | 1.94                     | 0.68              |
| 1:AA:1342:C:H2'   | 1:AA:1343:G:C8     | 2.28                     | 0.68              |
| 11:AL:8:ARG:CZ    | 11:AL:9:LYS:HE3    | 2.24                     | 0.68              |
| 12:AM:77:LYS:HA   | 12:AM:80:MET:HB3   | 1.74                     | 0.68              |
| 15:AP:68:SER:HB3  | 15:AP:71:VAL:HG12  | 1.76                     | 0.68              |
| 23:BB:303:G:H2'   | 23:BB:304:U:C6     | 2.29                     | 0.68              |
| 25:BC:20:ASN:HB3  | 25:BC:202:ARG:HB3  | 1.75                     | 0.68              |
| 26:BD:62:LYS:CD   | 26:BD:62:LYS:H     | 2.05                     | 0.68              |
| 35:BN:115:LEU:O   | 35:BN:116:VAL:HG12 | 1.92                     | 0.68              |
| 37:BP:21:PRO:HB2  | 37:BP:49:ILE:HD13  | 1.76                     | 0.68              |
| 3:CD:157:ALA:HA   | 3:CD:160:LEU:HD12  | 1.76                     | 0.68              |
| 4:CE:35:LEU:HD21  | 4:CE:136:VAL:HG21  | 1.75                     | 0.68              |
| 23:DB:1098:A:H3'  | 52:DI:3:LYS:HB3    | 1.76                     | 0.68              |
| 23:DB:1845:G:H4'  | 25:DC:268:ARG:HD3  | 1.76                     | 0.68              |
| 23:DB:2086:U:H2'  | 23:DB:2087:G:C8    | 2.29                     | 0.68              |
| 23:DB:2198:A:H4'  | 23:DB:2199:A:OP1   | 1.92                     | 0.68              |
| 25:DC:63:ILE:HG23 | 25:DC:102:TYR:CD1  | 2.28                     | 0.68              |
| 27:DE:138:LEU:O   | 27:DE:143:LEU:HD21 | 1.94                     | 0.68              |
| 31:DJ:68:LYS:HD2  | 31:DJ:72:LYS:HB2   | 1.76                     | 0.68              |
| 37:DP:50:ARG:NH1  | 37:DP:62:LYS:HB2   | 2.09                     | 0.68              |
| 48:D1:26:LYS:HE2  | 48:D1:28:THR:HB    | 1.76                     | 0.68              |
| 2:AC:71:ARG:HH21  | 2:AC:74:ILE:HB     | 1.57                     | 0.68              |
| 18:AS:7:GLY:H     | 18:AS:8:PRO:HD3    | 1.59                     | 0.68              |
| 23:BB:417:C:H2'   | 23:BB:418:C:C6     | 2.29                     | 0.68              |
| 23:BB:2575:C:H4'  | 26:BD:149:ASN:N    | 2.09                     | 0.68              |
| 23:BB:2621:G:O2'  | 26:BD:164:GLN:HB2  | 1.94                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:BD:148:GLN:HG3 | 26:BD:151:THR:OG1  | 1.93                     | 0.68              |
| 36:BO:48:LEU:HD23 | 36:BO:49:VAL:H     | 1.59                     | 0.68              |
| 38:BQ:47:ARG:NH2  | 38:BQ:50:ARG:HB3   | 2.09                     | 0.68              |
| 50:B3:23:HIS:CD2  | 50:B3:23:HIS:H     | 2.10                     | 0.68              |
| 1:CA:695:A:H5'    | 10:CK:52:ARG:HH22  | 1.58                     | 0.68              |
| 1:CA:947:G:H2'    | 1:CA:948:C:C6      | 2.29                     | 0.68              |
| 9:CJ:9:ARG:HB2    | 9:CJ:99:GLN:HG3    | 1.75                     | 0.68              |
| 20:CB:40:ILE:HG23 | 20:CB:200:PRO:HB2  | 1.76                     | 0.68              |
| 23:DB:117:G:H5'   | 23:DB:126:A:H8     | 1.58                     | 0.68              |
| 23:DB:162:U:H4'   | 23:DB:163:C:OP1    | 1.92                     | 0.68              |
| 23:DB:594:U:H2'   | 23:DB:595:C:C6     | 2.28                     | 0.68              |
| 23:DB:743:A:O2'   | 23:DB:744:U:H5'    | 1.93                     | 0.68              |
| 23:DB:2395:C:H2'  | 23:DB:2396:G:O4'   | 1.94                     | 0.68              |
| 23:DB:2849:U:H4'  | 23:DB:2850:A:H5'   | 1.74                     | 0.68              |
| 30:DH:54:LEU:HD23 | 30:DH:57:LYS:HD3   | 1.76                     | 0.68              |
| 32:DK:77:ILE:HD11 | 32:DK:105:ARG:NH1  | 2.09                     | 0.68              |
| 34:DM:16:ARG:HE   | 34:DM:18:ARG:NH1   | 1.92                     | 0.68              |
| 42:DU:28:LEU:HD11 | 42:DU:31:GLY:C     | 2.19                     | 0.68              |
| 44:DX:25:GLN:NE2  | 44:DX:29:ARG:HH21  | 1.92                     | 0.68              |
| 1:AA:865:A:H2'    | 1:AA:866:C:C6      | 2.28                     | 0.68              |
| 1:AA:1432:G:OP1   | 37:BP:105:LYS:HE3  | 1.94                     | 0.68              |
| 23:BB:580:U:H2'   | 23:BB:581:C:C6     | 2.29                     | 0.68              |
| 23:BB:1177:G:H2'  | 23:BB:1178:C:H6    | 1.59                     | 0.68              |
| 23:BB:2198:A:H4'  | 23:BB:2199:A:OP1   | 1.94                     | 0.68              |
| 23:BB:2395:C:H2'  | 23:BB:2396:G:O4'   | 1.94                     | 0.68              |
| 23:BB:2575:C:H5'' | 26:BD:149:ASN:HB3  | 1.75                     | 0.68              |
| 52:BI:5:GLN:HG2   | 52:BI:6:ALA:N      | 2.08                     | 0.68              |
| 1:CA:662:U:H2'    | 1:CA:663:A:C8      | 2.29                     | 0.68              |
| 4:CE:67:ARG:HB2   | 4:CE:67:ARG:HH11   | 1.59                     | 0.68              |
| 22:DA:61:G:H2'    | 22:DA:62:C:C6      | 2.28                     | 0.68              |
| 23:DB:543:G:H2'   | 23:DB:544:C:H4'    | 1.73                     | 0.68              |
| 23:DB:2039:U:H2'  | 23:DB:2040:G:C8    | 2.28                     | 0.68              |
| 23:DB:2262:U:O4   | 43:DW:12:GLY:HA2   | 1.93                     | 0.68              |
| 23:DB:2405:G:C5'  | 33:DL:70:LYS:HG3   | 2.23                     | 0.68              |
| 23:DB:2591:C:H2'  | 23:DB:2592:G:H8    | 1.59                     | 0.68              |
| 23:DB:2783:U:H2'  | 23:DB:2784:U:C6    | 2.29                     | 0.68              |
| 27:DE:115:GLN:HB3 | 27:DE:117:ARG:HH11 | 1.58                     | 0.68              |
| 46:DZ:59:ARG:HD3  | 46:DZ:63:ARG:HD3   | 1.76                     | 0.68              |
| 1:AA:78:A:H2'     | 1:AA:79:G:H8       | 1.59                     | 0.68              |
| 1:AA:1252:A:H2'   | 1:AA:1253:G:H5''   | 1.75                     | 0.68              |
| 15:AP:3:THR:HG22  | 15:AP:66:THR:HB    | 1.75                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 20:AB:116:LEU:HB3 | 20:AB:140:LEU:HD21 | 1.76                     | 0.68              |
| 23:BB:558:U:OP1   | 31:BJ:113:PRO:HG2  | 1.93                     | 0.68              |
| 26:BD:114:LYS:HE3 | 26:BD:196:ALA:HB2  | 1.76                     | 0.68              |
| 1:CA:1436:U:H2'   | 1:CA:1437:A:C8     | 2.28                     | 0.68              |
| 4:CE:44:ARG:HG2   | 4:CE:72:ASN:ND2    | 2.09                     | 0.68              |
| 13:CN:50:LEU:HD12 | 13:CN:51:PRO:HD3   | 1.76                     | 0.68              |
| 18:CS:62:THR:H    | 18:CS:65:MET:HE3   | 1.57                     | 0.68              |
| 20:CB:10:LYS:HB2  | 20:CB:211:LEU:HD21 | 1.76                     | 0.68              |
| 23:DB:794:A:H2'   | 23:DB:795:C:C6     | 2.29                     | 0.68              |
| 23:DB:1799:G:H4'  | 23:DB:1800:C:O5'   | 1.93                     | 0.68              |
| 23:DB:2064:C:H2'  | 23:DB:2065:C:H6    | 1.58                     | 0.68              |
| 27:DE:137:LYS:HA  | 27:DE:137:LYS:HZ2  | 1.57                     | 0.68              |
| 27:DE:154:ASP:OD1 | 27:DE:158:PHE:HB2  | 1.94                     | 0.68              |
| 29:DG:66:THR:O    | 29:DG:70:LEU:HD13  | 1.94                     | 0.68              |
| 37:DP:26:GLU:HB3  | 37:DP:46:VAL:HG13  | 1.75                     | 0.68              |
| 38:DQ:3:VAL:C     | 38:DQ:4:LYS:HD3    | 2.19                     | 0.68              |
| 43:DW:46:ALA:HB2  | 43:DW:77:LYS:HD3   | 1.76                     | 0.68              |
| 47:D0:47:TYR:HB3  | 47:D0:52:LYS:H     | 1.59                     | 0.68              |
| 50:D3:33:THR:C    | 50:D3:34:LYS:HD2   | 2.19                     | 0.68              |
| 2:AC:57:GLU:HB2   | 2:AC:64:ARG:HB2    | 1.75                     | 0.68              |
| 3:AD:156:ALA:O    | 3:AD:159:GLU:HG2   | 1.94                     | 0.68              |
| 4:AE:85:LYS:HE2   | 4:AE:92:ARG:NH1    | 2.08                     | 0.68              |
| 23:BB:240:C:H3'   | 23:BB:241:A:H5''   | 1.75                     | 0.68              |
| 23:BB:479:A:N3    | 23:BB:481:G:H5''   | 2.09                     | 0.68              |
| 23:BB:2783:U:H2'  | 23:BB:2784:U:C6    | 2.29                     | 0.68              |
| 24:BV:70:ILE:HD13 | 24:BV:70:ILE:N     | 2.09                     | 0.68              |
| 24:BV:76:ASP:HB2  | 34:BM:136:MET:CG   | 2.24                     | 0.68              |
| 25:BC:21:PRO:O    | 25:BC:202:ARG:HD2  | 1.93                     | 0.68              |
| 26:BD:16:THR:O    | 37:BP:80:VAL:HB    | 1.94                     | 0.68              |
| 31:BJ:13:ARG:HH11 | 31:BJ:13:ARG:HG3   | 1.59                     | 0.68              |
| 1:CA:865:A:H2'    | 1:CA:866:C:C6      | 2.28                     | 0.68              |
| 5:CF:42:TRP:HB2   | 5:CF:59:TYR:HB2    | 1.76                     | 0.68              |
| 22:DA:104:A:H2'   | 22:DA:105:G:O4'    | 1.94                     | 0.68              |
| 23:DB:528:A:C2    | 23:DB:2042:A:H2'   | 2.29                     | 0.68              |
| 23:DB:1373:A:H2'  | 23:DB:1374:G:O4'   | 1.92                     | 0.68              |
| 23:DB:2471:A:HO2' | 23:DB:2472:G:H8    | 1.40                     | 0.68              |
| 28:DF:177:ARG:C   | 28:DF:177:ARG:HE   | 2.01                     | 0.68              |
| 2:AC:184:ASN:HD22 | 2:AC:185:THR:H     | 1.42                     | 0.67              |
| 3:AD:94:GLU:HG3   | 3:AD:103:ARG:NH1   | 2.09                     | 0.67              |
| 11:AL:35:ARG:HG3  | 11:AL:36:VAL:H     | 1.58                     | 0.67              |
| 23:BB:2297:A:N6   | 23:BB:2319:G:H5''  | 2.09                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:2318:G:O2'   | 23:BB:2319:G:C2    | 2.47                     | 0.67              |
| 24:BV:66:ASP:HB3   | 24:BV:68:LYS:HG2   | 1.76                     | 0.67              |
| 41:BT:30:ILE:O     | 41:BT:84:TYR:HA    | 1.94                     | 0.67              |
| 48:B1:7:LYS:HD3    | 48:B1:24:LYS:HB2   | 1.76                     | 0.67              |
| 4:CE:22:LYS:HB3    | 4:CE:29:ILE:HB     | 1.75                     | 0.67              |
| 6:CG:25:PHE:HD1    | 6:CG:100:MET:HB2   | 1.59                     | 0.67              |
| 18:CS:62:THR:HG23  | 18:CS:63:ASP:H     | 1.59                     | 0.67              |
| 23:DB:2089:C:H2'   | 23:DB:2090:A:O4'   | 1.94                     | 0.67              |
| 23:DB:2334:U:H3    | 43:DW:74:LYS:CE    | 2.06                     | 0.67              |
| 23:DB:2743:U:H2'   | 23:DB:2744:G:H5''  | 1.75                     | 0.67              |
| 37:DP:64:SER:HA    | 37:DP:71:ARG:CB    | 2.23                     | 0.67              |
| 8:AI:112:ARG:HB2   | 8:AI:112:ARG:HH11  | 1.57                     | 0.67              |
| 14:AO:31:LEU:HD12  | 14:AO:58:MET:HB2   | 1.76                     | 0.67              |
| 19:AT:67:HIS:O     | 19:AT:70:LYS:HG2   | 1.93                     | 0.67              |
| 23:BB:598:U:H2'    | 23:BB:599:A:H8     | 1.58                     | 0.67              |
| 23:BB:1163:G:H21   | 39:BR:91:GLN:HG3   | 1.58                     | 0.67              |
| 23:BB:1531:C:H2'   | 23:BB:1532:A:C8    | 2.29                     | 0.67              |
| 23:BB:1917:U:H2'   | 23:BB:1918:A:H5'   | 1.76                     | 0.67              |
| 25:BC:42:ARG:CG    | 25:BC:43:ASN:H     | 2.01                     | 0.67              |
| 25:BC:144:GLU:HB2  | 25:BC:146:LYS:O    | 1.93                     | 0.67              |
| 26:BD:98:VAL:HA    | 26:BD:101:PHE:CZ   | 2.28                     | 0.67              |
| 26:BD:128:ARG:HH22 | 26:BD:130:GLN:HG3  | 1.60                     | 0.67              |
| 29:BG:85:LYS:O     | 29:BG:86:LEU:HD22  | 1.94                     | 0.67              |
| 32:BK:98:ARG:C     | 32:BK:99:ILE:HD12  | 2.20                     | 0.67              |
| 48:B1:29:LYS:HE3   | 48:B1:30:PRO:HD2   | 1.75                     | 0.67              |
| 48:B1:51:ALA:C     | 48:B1:52:LYS:HD2   | 2.18                     | 0.67              |
| 51:B4:14:CYS:HA    | 51:B4:26:ILE:O     | 1.93                     | 0.67              |
| 1:CA:1026:G:H2'    | 1:CA:1027:C:H6     | 1.60                     | 0.67              |
| 19:CT:34:VAL:HG11  | 19:CT:78:LEU:HD13  | 1.75                     | 0.67              |
| 20:CB:185:ILE:HA   | 20:CB:199:ILE:HG13 | 1.76                     | 0.67              |
| 23:DB:596:U:H2'    | 23:DB:597:G:H8     | 1.57                     | 0.67              |
| 23:DB:2143:C:H3'   | 23:DB:2144:G:H8    | 1.59                     | 0.67              |
| 26:DD:202:ILE:HG23 | 26:DD:204:LYS:HE3  | 1.76                     | 0.67              |
| 28:DF:151:LEU:HG   | 28:DF:153:ILE:HG13 | 1.74                     | 0.67              |
| 34:DM:100:LYS:O    | 34:DM:101:VAL:HG23 | 1.94                     | 0.67              |
| 43:DW:17:ALA:O     | 43:DW:18:LYS:HG2   | 1.95                     | 0.67              |
| 47:D0:52:LYS:O     | 47:D0:53:VAL:HG12  | 1.93                     | 0.67              |
| 1:AA:541:G:O2'     | 3:AD:39:GLN:HB2    | 1.93                     | 0.67              |
| 1:AA:1029:U:H5''   | 1:AA:1030:U:H5     | 1.59                     | 0.67              |
| 1:AA:1300:G:H1'    | 1:AA:1301:U:H5     | 1.59                     | 0.67              |
| 6:AG:66:GLU:HA     | 6:AG:69:ARG:HE     | 1.59                     | 0.67              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 13:AN:60:ARG:HD3  | 13:AN:60:ARG:N     | 2.05                     | 0.67              |
| 19:AT:15:LYS:HD3  | 19:AT:18:LYS:HE3   | 1.76                     | 0.67              |
| 23:BB:559:G:H1'   | 38:BQ:55:GLN:NE2   | 2.10                     | 0.67              |
| 23:BB:811:U:O2    | 23:BB:1250:G:H3'   | 1.95                     | 0.67              |
| 26:BD:89:GLU:HG2  | 26:BD:89:GLU:O     | 1.93                     | 0.67              |
| 27:BE:128:ALA:HB3 | 27:BE:129:PRO:CD   | 2.20                     | 0.67              |
| 38:BQ:39:ILE:O    | 38:BQ:43:GLN:HG3   | 1.94                     | 0.67              |
| 40:BS:34:ASP:H    | 40:BS:37:THR:CG2   | 2.06                     | 0.67              |
| 41:BT:54:GLU:N    | 41:BT:91:GLN:HE22  | 1.88                     | 0.67              |
| 1:CA:1306:A:N6    | 1:CA:1331:G:O2'    | 2.27                     | 0.67              |
| 2:CC:127:VAL:HG23 | 2:CC:128:MET:H     | 1.57                     | 0.67              |
| 23:DB:1060:U:O2   | 23:DB:1088:A:N7    | 2.27                     | 0.67              |
| 23:DB:1190:G:OP1  | 33:DL:38:GLN:HB2   | 1.94                     | 0.67              |
| 23:DB:1201:U:H2'  | 23:DB:1202:G:H8    | 1.59                     | 0.67              |
| 23:DB:2795:C:H2'  | 23:DB:2796:U:O4'   | 1.94                     | 0.67              |
| 31:DJ:35:ARG:HH12 | 31:DJ:40:HIS:N     | 1.82                     | 0.67              |
| 31:DJ:96:ARG:HD2  | 31:DJ:99:ARG:HH21  | 1.58                     | 0.67              |
| 33:DL:18:ARG:HH12 | 33:DL:21:ARG:HD3   | 1.59                     | 0.67              |
| 36:DO:66:GLY:N    | 36:DO:70:ALA:HB2   | 2.07                     | 0.67              |
| 37:DP:29:VAL:HG23 | 37:DP:47:ILE:HD11  | 1.76                     | 0.67              |
| 37:DP:112:ARG:H   | 37:DP:112:ARG:HE   | 1.41                     | 0.67              |
| 1:AA:987:G:H2'    | 1:AA:988:G:H8      | 1.60                     | 0.67              |
| 8:AI:34:LEU:HD11  | 8:AI:47:VAL:HG21   | 1.76                     | 0.67              |
| 20:AB:131:LYS:HA  | 20:AB:134:LEU:HD12 | 1.74                     | 0.67              |
| 23:BB:215:G:C4'   | 23:BB:216:A:H4'    | 2.25                     | 0.67              |
| 23:BB:417:C:H2'   | 23:BB:418:C:H6     | 1.59                     | 0.67              |
| 23:BB:596:U:H2'   | 23:BB:597:G:H8     | 1.58                     | 0.67              |
| 23:BB:2393:U:H5'' | 33:BL:62:PRO:HA    | 1.76                     | 0.67              |
| 25:BC:117:SER:HB3 | 25:BC:127:ASN:CG   | 2.19                     | 0.67              |
| 35:BN:100:CYS:HB3 | 35:BN:111:ALA:H    | 1.59                     | 0.67              |
| 43:BW:28:GLU:N    | 43:BW:61:LYS:HB2   | 2.09                     | 0.67              |
| 43:BW:35:ILE:HG12 | 43:BW:70:VAL:HG21  | 1.75                     | 0.67              |
| 46:BZ:5:ILE:HG23  | 46:BZ:63:ARG:HE    | 1.60                     | 0.67              |
| 49:B2:34:ARG:HE   | 49:B2:42:LEU:HD13  | 1.59                     | 0.67              |
| 51:B4:11:CYS:HB3  | 51:B4:14:CYS:SG    | 2.35                     | 0.67              |
| 52:BI:89:SER:HA   | 52:BI:97:VAL:CG2   | 2.25                     | 0.67              |
| 1:CA:194:C:O2'    | 1:CA:195:A:H5'     | 1.94                     | 0.67              |
| 1:CA:555:U:H2'    | 1:CA:556:C:H6      | 1.60                     | 0.67              |
| 3:CD:87:GLU:HG2   | 3:CD:187:ARG:HD3   | 1.76                     | 0.67              |
| 19:CT:66:ILE:HG13 | 19:CT:70:LYS:HE2   | 1.75                     | 0.67              |
| 23:DB:863:A:H2'   | 23:DB:864:G:H8     | 1.58                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:1533:C:O2'   | 23:DB:1534:U:H5'   | 1.95                     | 0.67              |
| 25:DC:87:SER:O     | 25:DC:157:ALA:HB2  | 1.95                     | 0.67              |
| 25:DC:260:LYS:HG2  | 25:DC:262:THR:OG1  | 1.95                     | 0.67              |
| 31:DJ:98:GLU:HG3   | 31:DJ:126:ALA:HB2  | 1.75                     | 0.67              |
| 41:DT:66:LYS:H     | 41:DT:76:ARG:NH2   | 1.90                     | 0.67              |
| 48:D1:46:VAL:HG22  | 48:D1:47:ILE:H     | 1.59                     | 0.67              |
| 51:D4:26:ILE:CD1   | 51:D4:34:LYS:HA    | 2.23                     | 0.67              |
| 1:AA:1320:C:N4     | 18:AS:35:ARG:HD3   | 2.10                     | 0.67              |
| 1:AA:1479:C:H2'    | 1:AA:1480:A:H8     | 1.59                     | 0.67              |
| 9:AJ:80:THR:HG22   | 9:AJ:81:GLU:H      | 1.60                     | 0.67              |
| 11:AL:19:ASN:O     | 11:AL:20:VAL:HG23  | 1.95                     | 0.67              |
| 23:BB:478:A:N1     | 23:BB:500:G:H4'    | 2.09                     | 0.67              |
| 23:BB:794:A:H2'    | 23:BB:795:C:C6     | 2.29                     | 0.67              |
| 23:BB:2750:A:H3'   | 29:BG:3:VAL:CG1    | 2.24                     | 0.67              |
| 30:BH:6:LEU:HA     | 30:BH:15:LEU:CA    | 2.24                     | 0.67              |
| 36:BO:67:ASN:HA    | 36:BO:71:ALA:HB3   | 1.75                     | 0.67              |
| 38:BQ:52:ARG:CZ    | 38:BQ:55:GLN:HG2   | 2.24                     | 0.67              |
| 22:DA:49:C:H4'     | 36:DO:68:LYS:HZ3   | 1.59                     | 0.67              |
| 23:DB:594:U:H2'    | 23:DB:595:C:H6     | 1.60                     | 0.67              |
| 23:DB:1341:G:H5'   | 41:DT:61:LEU:HD21  | 1.76                     | 0.67              |
| 23:DB:1437:C:H2'   | 23:DB:1438:U:H6    | 1.60                     | 0.67              |
| 23:DB:1534:U:HO2'  | 23:DB:1535:A:H8    | 1.40                     | 0.67              |
| 29:DG:36:LEU:HB2   | 29:DG:40:VAL:HG21  | 1.76                     | 0.67              |
| 32:DK:43:ILE:H     | 32:DK:43:ILE:HD12  | 1.58                     | 0.67              |
| 33:DL:58:TYR:HB3   | 50:D3:13:PHE:CZ    | 2.30                     | 0.67              |
| 44:DX:12:GLU:HG2   | 44:DX:12:GLU:O     | 1.94                     | 0.67              |
| 51:D4:26:ILE:CG1   | 51:D4:35:GLN:H     | 2.02                     | 0.67              |
| 23:BB:445:C:OP1    | 38:BQ:1:ALA:HB3    | 1.94                     | 0.67              |
| 23:BB:2804:U:H2'   | 23:BB:2805:C:H6    | 1.58                     | 0.67              |
| 23:BB:2834:G:H1'   | 23:BB:2883:A:H61   | 1.58                     | 0.67              |
| 26:BD:138:LEU:H    | 26:BD:138:LEU:CD2  | 2.07                     | 0.67              |
| 27:BE:60:TRP:NE1   | 27:BE:73:ILE:HD11  | 2.08                     | 0.67              |
| 27:BE:164:LEU:O    | 27:BE:165:HIS:HB2  | 1.93                     | 0.67              |
| 28:BF:59:ILE:HD11  | 28:BF:137:PHE:CD2  | 2.28                     | 0.67              |
| 41:BT:36:LYS:HD3   | 41:BT:36:LYS:C     | 2.20                     | 0.67              |
| 44:BX:55:THR:HG22  | 44:BX:59:GLU:OE1   | 1.95                     | 0.67              |
| 51:B4:20:ASP:OD2   | 51:B4:22:VAL:HG13  | 1.93                     | 0.67              |
| 20:CB:206:ILE:HG22 | 20:CB:207:ARG:HH21 | 1.57                     | 0.67              |
| 23:DB:479:A:O2'    | 23:DB:481:G:H5'    | 1.95                     | 0.67              |
| 23:DB:833:A:H2'    | 23:DB:834:G:C8     | 2.30                     | 0.67              |
| 23:DB:2088:A:H2'   | 23:DB:2089:C:C6    | 2.28                     | 0.67              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DB:2266:A:H4'  | 23:DB:2267:A:C2   | 2.30                     | 0.67              |
| 23:DB:2880:C:H1'  | 35:DN:92:GLY:O    | 1.95                     | 0.67              |
| 29:DG:16:VAL:HG22 | 29:DG:25:ILE:HG13 | 1.77                     | 0.67              |
| 34:DM:71:LYS:HB2  | 34:DM:72:PRO:HD3  | 1.75                     | 0.67              |
| 34:DM:118:LYS:HB2 | 34:DM:118:LYS:NZ  | 2.09                     | 0.67              |
| 38:DQ:26:ALA:HA   | 38:DQ:30:VAL:HG23 | 1.76                     | 0.67              |
| 41:DT:55:VAL:HG23 | 41:DT:87:LEU:H    | 1.59                     | 0.67              |
| 4:AE:83:PRO:HB3   | 4:AE:96:GLN:HG3   | 1.76                     | 0.67              |
| 4:AE:110:MET:HB3  | 4:AE:139:THR:HG21 | 1.76                     | 0.67              |
| 15:AP:9:HIS:HE1   | 15:AP:29:ASN:HB2  | 1.59                     | 0.67              |
| 23:BB:282:A:H2'   | 23:BB:283:G:C8    | 2.30                     | 0.67              |
| 23:BB:587:C:OP2   | 33:BL:29:LYS:HA   | 1.94                     | 0.67              |
| 23:BB:1250:G:O2'  | 23:BB:1251:C:OP1  | 2.12                     | 0.67              |
| 23:BB:1486:U:H2'  | 23:BB:1487:U:H6   | 1.59                     | 0.67              |
| 23:BB:2769:U:H2'  | 23:BB:2770:G:H8   | 1.58                     | 0.67              |
| 23:BB:2836:U:H2'  | 23:BB:2837:A:H8   | 1.60                     | 0.67              |
| 25:BC:21:PRO:HG2  | 25:BC:202:ARG:NH1 | 2.09                     | 0.67              |
| 25:BC:79:ARG:CZ   | 25:BC:110:LYS:HD3 | 2.24                     | 0.67              |
| 27:BE:17:THR:HA   | 27:BE:199:MET:HG3 | 1.76                     | 0.67              |
| 28:BF:9:ASP:O     | 28:BF:10:GLU:HB2  | 1.93                     | 0.67              |
| 39:BR:46:GLU:O    | 39:BR:47:VAL:HB   | 1.95                     | 0.67              |
| 41:BT:38:ALA:O    | 41:BT:42:GLU:HB2  | 1.95                     | 0.67              |
| 42:BU:4:ILE:O     | 42:BU:27:VAL:HG11 | 1.95                     | 0.67              |
| 1:CA:1296:C:H4'   | 1:CA:1302:C:H41   | 1.60                     | 0.67              |
| 5:CF:3:HIS:HB3    | 5:CF:92:THR:CA    | 2.22                     | 0.67              |
| 11:CL:93:ARG:H    | 11:CL:93:ARG:HD2  | 1.59                     | 0.67              |
| 20:CB:16:GLY:HA2  | 20:CB:40:ILE:HG13 | 1.77                     | 0.67              |
| 20:CB:27:LYS:HB3  | 20:CB:28:PRO:HD3  | 1.77                     | 0.67              |
| 23:DB:598:U:H2'   | 23:DB:599:A:H8    | 1.58                     | 0.67              |
| 23:DB:2278:A:H62  | 43:DW:10:ARG:HB2  | 1.59                     | 0.67              |
| 23:DB:2292:U:H2'  | 23:DB:2293:G:H8   | 1.60                     | 0.67              |
| 23:DB:2391:G:OP2  | 50:D3:32:LEU:HG   | 1.95                     | 0.67              |
| 23:DB:2769:U:H2'  | 23:DB:2770:G:H8   | 1.58                     | 0.67              |
| 25:DC:20:ASN:HB2  | 25:DC:202:ARG:NH1 | 2.10                     | 0.67              |
| 26:DD:122:VAL:HA  | 26:DD:128:ARG:CG  | 2.24                     | 0.67              |
| 28:DF:18:GLU:C    | 28:DF:20:ASN:H    | 2.03                     | 0.67              |
| 29:DG:55:ASP:CG   | 29:DG:56:GLY:H    | 2.02                     | 0.67              |
| 41:DT:55:VAL:HG22 | 41:DT:56:GLU:N    | 2.08                     | 0.67              |
| 1:AA:1170:A:H2'   | 1:AA:1171:A:O4'   | 1.94                     | 0.67              |
| 1:AA:1313:U:H5''  | 18:AS:5:LYS:CG    | 2.24                     | 0.67              |
| 5:AF:12:PRO:HG3   | 5:AF:54:LEU:HG    | 1.76                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:AT:48:LYS:O     | 19:AT:52:GLU:HB2   | 1.95                     | 0.67              |
| 20:AB:212:TYR:O    | 20:AB:216:VAL:HG23 | 1.94                     | 0.67              |
| 23:BB:329:G:O6     | 42:BU:16:LYS:HB2   | 1.95                     | 0.67              |
| 23:BB:589:U:H2'    | 23:BB:590:A:C8     | 2.30                     | 0.67              |
| 23:BB:643:A:N6     | 23:BB:2370:G:H1'   | 2.10                     | 0.67              |
| 23:BB:751:A:H5'    | 40:BS:90:LYS:HE3   | 1.75                     | 0.67              |
| 25:BC:9:SER:HB2    | 25:BC:202:ARG:CZ   | 2.25                     | 0.67              |
| 25:BC:238:ASN:HB3  | 25:BC:242:HIS:NE2  | 2.09                     | 0.67              |
| 26:BD:146:ILE:HD12 | 26:BD:146:ILE:N    | 2.10                     | 0.67              |
| 27:BE:170:ARG:HH21 | 27:BE:175:ILE:HD12 | 1.59                     | 0.67              |
| 32:BK:26:GLY:HA3   | 32:BK:30:ARG:NE    | 2.06                     | 0.67              |
| 1:CA:398:U:H2'     | 1:CA:399:G:H8      | 1.60                     | 0.67              |
| 1:CA:554:A:H5'     | 11:CL:25:ALA:HB1   | 1.77                     | 0.67              |
| 2:CC:8:GLY:HA3     | 13:CN:88:MET:SD    | 2.35                     | 0.67              |
| 12:CM:79:LEU:HD22  | 12:CM:86:ARG:HE    | 1.60                     | 0.67              |
| 20:CB:202:ASN:HD22 | 20:CB:203:ASP:H    | 1.43                     | 0.67              |
| 23:DB:836:G:H2'    | 23:DB:837:C:H6     | 1.58                     | 0.67              |
| 23:DB:1531:C:H2'   | 23:DB:1532:A:C8    | 2.29                     | 0.67              |
| 23:DB:2900:A:H2'   | 23:DB:2901:C:C6    | 2.30                     | 0.67              |
| 25:DC:22:GLU:HB2   | 25:DC:202:ARG:CD   | 2.25                     | 0.67              |
| 27:DE:6:LYS:HD3    | 27:DE:7:ASP:N      | 2.10                     | 0.67              |
| 28:DF:39:VAL:HG22  | 28:DF:84:ILE:HD13  | 1.77                     | 0.67              |
| 29:DG:40:VAL:HG22  | 29:DG:51:PHE:CE2   | 2.29                     | 0.67              |
| 30:DH:6:LEU:CD1    | 30:DH:36:ALA:H     | 2.03                     | 0.67              |
| 34:DM:80:VAL:HG12  | 34:DM:81:ARG:H     | 1.60                     | 0.67              |
| 40:DS:73:LYS:HD3   | 40:DS:74:ILE:H     | 1.58                     | 0.67              |
| 44:DX:51:ALA:O     | 44:DX:53:VAL:N     | 2.28                     | 0.67              |
| 52:DI:27:LEU:H     | 52:DI:27:LEU:CD2   | 2.07                     | 0.67              |
| 1:AA:203:G:H1'     | 1:AA:465:A:H62     | 1.59                     | 0.67              |
| 1:AA:764:C:H3'     | 1:AA:765:G:N2      | 2.06                     | 0.67              |
| 1:AA:1219:A:H2'    | 1:AA:1220:G:H8     | 1.59                     | 0.67              |
| 6:AG:149:ALA:HB1   | 10:AK:58:THR:HG21  | 1.77                     | 0.67              |
| 8:AI:82:ILE:O      | 8:AI:86:LEU:HD22   | 1.95                     | 0.67              |
| 23:BB:721:A:H2'    | 23:BB:722:A:C8     | 2.29                     | 0.67              |
| 23:BB:1007:C:H5''  | 31:BJ:37:ARG:HH21  | 1.59                     | 0.67              |
| 23:BB:1210:G:H5'   | 23:BB:1212:G:O4'   | 1.95                     | 0.67              |
| 23:BB:2039:U:H2'   | 23:BB:2040:G:C8    | 2.28                     | 0.67              |
| 23:BB:2294:G:O2'   | 23:BB:2295:C:H5'   | 1.95                     | 0.67              |
| 30:BH:89:LYS:C     | 30:BH:90:LEU:HD12  | 2.20                     | 0.67              |
| 31:BJ:7:LYS:HZ3    | 31:BJ:49:ASP:H     | 1.43                     | 0.67              |
| 34:BM:35:ALA:O     | 34:BM:36:VAL:HG22  | 1.95                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:BZ:36:VAL:CA    | 46:BZ:42:PRO:HB3   | 2.23                     | 0.67              |
| 52:BI:77:VAL:HA    | 52:BI:80:LYS:HE2   | 1.76                     | 0.67              |
| 1:CA:763:G:H2'     | 1:CA:764:C:H6      | 1.60                     | 0.67              |
| 12:CM:39:ALA:O     | 12:CM:42:VAL:HG22  | 1.94                     | 0.67              |
| 23:DB:1568:G:OP1   | 25:DC:61:TYR:HB2   | 1.95                     | 0.67              |
| 26:DD:48:ILE:HA    | 26:DD:80:TRP:HB3   | 1.77                     | 0.67              |
| 26:DD:130:GLN:HB3  | 26:DD:140:HIS:HA   | 1.77                     | 0.67              |
| 33:DL:34:GLY:HA3   | 39:DR:85:LYS:HG2   | 1.77                     | 0.67              |
| 37:DP:7:LEU:HD23   | 37:DP:11:GLN:HE21  | 1.60                     | 0.67              |
| 39:DR:47:VAL:CG1   | 39:DR:49:ILE:HG12  | 2.25                     | 0.67              |
| 43:DW:42:THR:HB    | 43:DW:75:ASN:CB    | 2.24                     | 0.67              |
| 1:AA:586:C:O2'     | 1:AA:587:G:H5'     | 1.94                     | 0.67              |
| 1:AA:1218:C:H2'    | 1:AA:1219:A:H8     | 1.59                     | 0.67              |
| 5:AF:53:LYS:HA     | 5:AF:53:LYS:NZ     | 2.09                     | 0.67              |
| 7:AH:29:SER:HB3    | 7:AH:32:LYS:HG3    | 1.77                     | 0.67              |
| 10:AK:110:THR:HG21 | 21:AU:4:LYS:HD2    | 1.77                     | 0.67              |
| 11:AL:20:VAL:HG13  | 11:AL:94:TYR:OH    | 1.95                     | 0.67              |
| 16:AQ:29:LYS:HD3   | 16:AQ:35:LYS:N     | 2.10                     | 0.67              |
| 23:BB:442:G:N2     | 27:BE:46:GLN:NE2   | 2.44                     | 0.67              |
| 23:BB:1410:G:H2'   | 23:BB:1411:U:C6    | 2.29                     | 0.67              |
| 23:BB:2537:U:H2'   | 23:BB:2538:C:H6    | 1.60                     | 0.67              |
| 34:BM:3:GLN:O      | 34:BM:5:LYS:N      | 2.28                     | 0.67              |
| 35:BN:114:GLU:HG2  | 35:BN:115:LEU:H    | 1.59                     | 0.67              |
| 43:BW:2:HIS:C      | 43:BW:3:LYS:HD2    | 2.20                     | 0.67              |
| 50:B3:41:ARG:HB3   | 50:B3:43:LEU:HD22  | 1.77                     | 0.67              |
| 1:CA:555:U:H2'     | 1:CA:556:C:C6      | 2.30                     | 0.67              |
| 1:CA:673:A:H2'     | 1:CA:674:G:C8      | 2.28                     | 0.67              |
| 1:CA:918:A:H2'     | 1:CA:919:A:C8      | 2.30                     | 0.67              |
| 1:CA:1202:U:H1'    | 13:CN:68:ARG:HD2   | 1.77                     | 0.67              |
| 9:CJ:12:ALA:HB3    | 9:CJ:18:ILE:HB     | 1.75                     | 0.67              |
| 20:CB:103:TRP:O    | 20:CB:107:ARG:HG3  | 1.95                     | 0.67              |
| 22:DA:26:C:H2'     | 22:DA:27:C:C6      | 2.29                     | 0.67              |
| 25:DC:107:LYS:CE   | 25:DC:108:GLY:H    | 2.05                     | 0.67              |
| 27:DE:138:LEU:HD22 | 27:DE:187:VAL:HG11 | 1.75                     | 0.67              |
| 39:DR:74:ILE:O     | 39:DR:75:VAL:HG13  | 1.94                     | 0.67              |
| 1:AA:398:U:H2'     | 1:AA:399:G:H8      | 1.60                     | 0.66              |
| 1:AA:555:U:H2'     | 1:AA:556:C:C6      | 2.30                     | 0.66              |
| 1:AA:1065:U:H1'    | 1:AA:1066:C:OP2    | 1.96                     | 0.66              |
| 1:AA:1193:G:O2'    | 1:AA:1194:U:H5'    | 1.95                     | 0.66              |
| 9:AJ:10:LEU:HG     | 9:AJ:98:VAL:HG12   | 1.76                     | 0.66              |
| 13:AN:50:LEU:HD23  | 13:AN:51:PRO:HD3   | 1.77                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:833:A:H2'    | 23:BB:834:G:C8     | 2.30                     | 0.66              |
| 26:BD:34:VAL:HG13  | 26:BD:89:GLU:OE2   | 1.94                     | 0.66              |
| 35:BN:72:ASP:HB3   | 35:BN:74:GLU:HG3   | 1.76                     | 0.66              |
| 1:CA:408:A:OP1     | 3:CD:111:ALA:HB3   | 1.95                     | 0.66              |
| 1:CA:538:G:OP2     | 11:CL:111:GLN:HB2  | 1.94                     | 0.66              |
| 1:CA:678:U:H2'     | 1:CA:679:C:C6      | 2.30                     | 0.66              |
| 1:CA:678:U:H2'     | 1:CA:679:C:H6      | 1.59                     | 0.66              |
| 5:CF:68:GLN:HA     | 5:CF:71:ILE:HG22   | 1.77                     | 0.66              |
| 6:CG:70:PRO:HA     | 6:CG:141:HIS:HE1   | 1.59                     | 0.66              |
| 11:CL:65:TYR:HB2   | 11:CL:92:VAL:HG11  | 1.77                     | 0.66              |
| 23:DB:1799:G:H5''  | 25:DC:255:LYS:HE3  | 1.76                     | 0.66              |
| 23:DB:2723:C:H5'   | 35:DN:4:ARG:CZ     | 2.25                     | 0.66              |
| 23:DB:2836:U:H2'   | 23:DB:2837:A:H8    | 1.60                     | 0.66              |
| 26:DD:122:VAL:HG22 | 26:DD:128:ARG:HG3  | 1.77                     | 0.66              |
| 31:DJ:37:ARG:HH21  | 31:DJ:46:PRO:HB3   | 1.59                     | 0.66              |
| 36:DO:82:ALA:C     | 36:DO:87:ILE:HG21  | 2.20                     | 0.66              |
| 46:DZ:49:ARG:C     | 46:DZ:51:VAL:H     | 2.03                     | 0.66              |
| 1:AA:662:U:H2'     | 1:AA:663:A:C8      | 2.30                     | 0.66              |
| 1:AA:763:G:H2'     | 1:AA:764:C:H6      | 1.59                     | 0.66              |
| 16:AQ:75:VAL:HG23  | 16:AQ:76:ARG:H     | 1.59                     | 0.66              |
| 23:BB:1082:U:N3    | 23:BB:1086:A:C6    | 2.63                     | 0.66              |
| 23:BB:2147:A:H5'   | 23:BB:2148:G:C4'   | 2.26                     | 0.66              |
| 23:BB:2527:C:H1'   | 51:B4:1:MET:HB3    | 1.77                     | 0.66              |
| 23:BB:2591:C:H2'   | 23:BB:2592:G:H8    | 1.59                     | 0.66              |
| 35:BN:97:ILE:CD1   | 35:BN:113:ILE:HD13 | 2.24                     | 0.66              |
| 39:BR:5:PHE:HA     | 39:BR:40:MET:CG    | 2.25                     | 0.66              |
| 46:BZ:55:GLY:HA2   | 46:BZ:63:ARG:HG3   | 1.78                     | 0.66              |
| 1:CA:909:A:H2'     | 1:CA:910:C:O4'     | 1.95                     | 0.66              |
| 3:CD:30:LYS:HZ2    | 3:CD:30:LYS:HB2    | 1.59                     | 0.66              |
| 4:CE:87:VAL:HG22   | 4:CE:88:HIS:N      | 2.09                     | 0.66              |
| 8:CI:98:ARG:HA     | 8:CI:103:VAL:HG22  | 1.75                     | 0.66              |
| 9:CJ:8:ILE:HA      | 9:CJ:100:ILE:HG22  | 1.76                     | 0.66              |
| 9:CJ:48:ARG:HB3    | 9:CJ:66:GLU:HG3    | 1.78                     | 0.66              |
| 11:CL:54:VAL:HG11  | 11:CL:79:ILE:HD11  | 1.77                     | 0.66              |
| 15:CP:61:VAL:HA    | 15:CP:65:ALA:HB3   | 1.77                     | 0.66              |
| 21:CU:48:LYS:HA    | 21:CU:51:ALA:HB3   | 1.77                     | 0.66              |
| 23:DB:532:A:H4'    | 23:DB:533:G:C8     | 2.30                     | 0.66              |
| 23:DB:1410:G:H2'   | 23:DB:1411:U:C6    | 2.29                     | 0.66              |
| 23:DB:1486:U:H2'   | 23:DB:1487:U:H6    | 1.59                     | 0.66              |
| 24:DV:48:MET:HE1   | 24:DV:85:LYS:HA    | 1.77                     | 0.66              |
| 30:DH:87:GLU:HB2   | 30:DH:89:LYS:NZ    | 2.08                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:DJ:132:HIS:HB3  | 31:DJ:136:GLN:OE1  | 1.95                     | 0.66              |
| 32:DK:19:VAL:HG12  | 32:DK:43:ILE:HA    | 1.77                     | 0.66              |
| 37:DP:36:LYS:HG2   | 37:DP:37:LYS:HE3   | 1.76                     | 0.66              |
| 42:DU:17:ASP:OD2   | 42:DU:20:LYS:HB2   | 1.95                     | 0.66              |
| 42:DU:82:VAL:HB    | 42:DU:94:PHE:HB3   | 1.76                     | 0.66              |
| 48:D1:16:THR:HG22  | 48:D1:47:ILE:HD12  | 1.77                     | 0.66              |
| 51:D4:34:LYS:HE2   | 51:D4:36:ARG:NH2   | 2.10                     | 0.66              |
| 1:AA:678:U:H2'     | 1:AA:679:C:C6      | 2.30                     | 0.66              |
| 1:AA:1116:U:O2'    | 1:AA:1117:A:H5'    | 1.95                     | 0.66              |
| 23:BB:1132:U:C5'   | 31:BJ:85:LYS:HZ3   | 2.08                     | 0.66              |
| 23:BB:1212:G:O2'   | 23:BB:1236:G:N2    | 2.27                     | 0.66              |
| 23:BB:1437:C:H2'   | 23:BB:1438:U:H6    | 1.59                     | 0.66              |
| 23:BB:2471:A:HO2'  | 23:BB:2472:G:H8    | 1.37                     | 0.66              |
| 23:BB:2511:U:O2'   | 26:BD:144:GLY:HA3  | 1.94                     | 0.66              |
| 26:BD:165:MET:HE3  | 26:BD:166:GLY:H    | 1.60                     | 0.66              |
| 27:BE:117:ARG:H    | 27:BE:118:LEU:HD23 | 1.60                     | 0.66              |
| 31:BJ:56:VAL:HB    | 31:BJ:124:VAL:HA   | 1.77                     | 0.66              |
| 35:BN:34:ILE:N     | 35:BN:34:ILE:HD13  | 2.10                     | 0.66              |
| 40:BS:103:ILE:HG13 | 40:BS:105:VAL:HG23 | 1.76                     | 0.66              |
| 1:CA:731:G:H5'     | 1:CA:766:A:H4'     | 1.78                     | 0.66              |
| 1:CA:1078:U:H4'    | 4:CE:137:ARG:NH1   | 2.10                     | 0.66              |
| 1:CA:1270:G:H2'    | 1:CA:1271:A:H8     | 1.61                     | 0.66              |
| 6:CG:2:ARG:NH1     | 6:CG:2:ARG:HB3     | 2.10                     | 0.66              |
| 8:CI:29:ILE:HA     | 8:CI:64:ILE:HB     | 1.76                     | 0.66              |
| 23:DB:1456:G:O2'   | 23:DB:1457:U:H5'   | 1.95                     | 0.66              |
| 23:DB:2243:U:H2'   | 23:DB:2244:U:C6    | 2.30                     | 0.66              |
| 23:DB:2286:G:H1    | 48:D1:23:THR:HG21  | 1.60                     | 0.66              |
| 25:DC:20:ASN:CG    | 25:DC:202:ARG:HD3  | 2.20                     | 0.66              |
| 26:DD:125:TRP:HB2  | 26:DD:160:LYS:CD   | 2.25                     | 0.66              |
| 39:DR:6:GLN:HG2    | 39:DR:7:SER:H      | 1.60                     | 0.66              |
| 42:DU:42:LYS:H     | 42:DU:57:ILE:HD12  | 1.58                     | 0.66              |
| 43:DW:31:LEU:HD22  | 43:DW:39:GLN:HE22  | 1.61                     | 0.66              |
| 1:AA:72:A:H2'      | 1:AA:73:C:H6       | 1.60                     | 0.66              |
| 1:AA:1008:U:H2'    | 1:AA:1009:U:C4'    | 2.25                     | 0.66              |
| 1:AA:1163:A:H2'    | 1:AA:1164:G:H8     | 1.60                     | 0.66              |
| 2:AC:5:HIS:CD2     | 13:AN:88:MET:HB3   | 2.30                     | 0.66              |
| 3:AD:2:ARG:HG3     | 3:AD:114:ARG:CZ    | 2.26                     | 0.66              |
| 23:BB:161:A:H62    | 23:BB:165:A:H61    | 1.41                     | 0.66              |
| 23:BB:1714:U:H3'   | 23:BB:1715:G:H5'   | 1.77                     | 0.66              |
| 27:BE:148:ILE:HB   | 27:BE:185:LYS:O    | 1.95                     | 0.66              |
| 29:BG:40:VAL:HG21  | 29:BG:53:PRO:HA    | 1.76                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:BJ:23:LYS:H    | 31:BJ:23:LYS:HD2   | 1.61                     | 0.66              |
| 43:BW:66:VAL:HG22 | 43:BW:67:LYS:N     | 2.11                     | 0.66              |
| 1:CA:16:A:O2'     | 1:CA:17:U:H5'      | 1.96                     | 0.66              |
| 1:CA:376:G:H5''   | 15:CP:5:ARG:HB2    | 1.76                     | 0.66              |
| 9:CJ:37:ARG:HB2   | 9:CJ:76:ILE:HA     | 1.75                     | 0.66              |
| 23:DB:857:G:H2'   | 23:DB:858:G:H5'    | 1.78                     | 0.66              |
| 23:DB:1082:U:N3   | 23:DB:1086:A:C6    | 2.62                     | 0.66              |
| 23:DB:2323:G:O2'  | 23:DB:2324:U:H5'   | 1.94                     | 0.66              |
| 23:DB:2531:A:OP1  | 29:DG:176:LYS:HA   | 1.95                     | 0.66              |
| 24:DV:4:ILE:O     | 24:DV:63:ILE:HA    | 1.95                     | 0.66              |
| 25:DC:74:PRO:HB2  | 25:DC:96:LYS:HG3   | 1.78                     | 0.66              |
| 26:DD:4:LEU:HD22  | 26:DD:51:THR:HB    | 1.76                     | 0.66              |
| 27:DE:6:LYS:HZ3   | 27:DE:8:ALA:HB2    | 1.59                     | 0.66              |
| 27:DE:105:LEU:O   | 27:DE:108:ILE:HG23 | 1.95                     | 0.66              |
| 29:DG:8:VAL:HB    | 29:DG:49:LEU:HB2   | 1.77                     | 0.66              |
| 2:AC:77:GLY:HA3   | 2:AC:82:ASP:H      | 1.61                     | 0.66              |
| 18:AS:49:ALA:HA   | 18:AS:57:VAL:O     | 1.96                     | 0.66              |
| 23:BB:469:G:OP2   | 27:BE:55:SER:HB2   | 1.96                     | 0.66              |
| 23:BB:1381:G:C2'  | 23:BB:1382:G:H5'   | 2.26                     | 0.66              |
| 23:BB:1843:C:O4'  | 25:BC:250:GLN:HG2  | 1.95                     | 0.66              |
| 23:BB:2270:A:H4'  | 43:BW:18:LYS:HG2   | 1.78                     | 0.66              |
| 26:BD:16:THR:C    | 37:BP:80:VAL:HB    | 2.20                     | 0.66              |
| 27:BE:5:LEU:HD12  | 27:BE:5:LEU:H      | 1.60                     | 0.66              |
| 33:BL:118:THR:H   | 33:BL:119:PRO:CD   | 2.06                     | 0.66              |
| 34:BM:8:LYS:HZ2   | 34:BM:70:ASP:N     | 1.92                     | 0.66              |
| 37:BP:29:VAL:O    | 37:BP:31:VAL:HG23  | 1.95                     | 0.66              |
| 52:BI:11:GLN:HA   | 52:BI:55:PRO:HA    | 1.76                     | 0.66              |
| 1:CA:56:U:H2'     | 1:CA:57:G:H8       | 1.61                     | 0.66              |
| 1:CA:239:U:H6     | 1:CA:239:U:C5'     | 2.08                     | 0.66              |
| 1:CA:812:G:HO2'   | 1:CA:813:U:H6      | 1.42                     | 0.66              |
| 6:CG:113:LYS:HE2  | 6:CG:113:LYS:HA    | 1.75                     | 0.66              |
| 6:CG:144:ALA:C    | 6:CG:146:ALA:H     | 2.04                     | 0.66              |
| 12:CM:74:MET:HE2  | 12:CM:77:LYS:HD2   | 1.78                     | 0.66              |
| 23:DB:2147:A:N3   | 23:DB:2147:A:H2'   | 2.11                     | 0.66              |
| 23:DB:2758:A:C2'  | 23:DB:2759:G:H5'   | 2.25                     | 0.66              |
| 24:DV:9:ARG:NH1   | 24:DV:12:GLN:HA    | 2.09                     | 0.66              |
| 26:DD:35:THR:HB   | 26:DD:48:ILE:HB    | 1.77                     | 0.66              |
| 26:DD:114:LYS:HB2 | 26:DD:114:LYS:NZ   | 2.10                     | 0.66              |
| 29:DG:4:ALA:O     | 29:DG:5:LYS:HB2    | 1.93                     | 0.66              |
| 29:DG:153:PRO:HA  | 29:DG:159:LYS:O    | 1.94                     | 0.66              |
| 34:DM:5:LYS:HD3   | 34:DM:71:LYS:HG2   | 1.77                     | 0.66              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 37:DP:90:ALA:HB3   | 37:DP:112:ARG:N   | 2.11                     | 0.66              |
| 38:DQ:57:ARG:HH21  | 38:DQ:92:LYS:HZ3  | 1.43                     | 0.66              |
| 39:DR:6:GLN:HG2    | 39:DR:7:SER:N     | 2.10                     | 0.66              |
| 49:D2:13:ASN:OD1   | 49:D2:17:GLY:HA3  | 1.96                     | 0.66              |
| 1:AA:678:U:H2'     | 1:AA:679:C:H6     | 1.59                     | 0.66              |
| 1:AA:922:G:H2'     | 1:AA:923:A:C8     | 2.31                     | 0.66              |
| 1:AA:1391:U:H2'    | 1:AA:1392:G:C8    | 2.31                     | 0.66              |
| 15:AP:46:LYS:CD    | 15:AP:46:LYS:H    | 2.08                     | 0.66              |
| 23:BB:163:C:H2'    | 23:BB:164:C:O4'   | 1.95                     | 0.66              |
| 23:BB:320:A:H4'    | 23:BB:322:A:N7    | 2.11                     | 0.66              |
| 23:BB:448:U:H1'    | 27:BE:79:ARG:HG3  | 1.76                     | 0.66              |
| 23:BB:545:U:H2'    | 23:BB:547:A:OP2   | 1.94                     | 0.66              |
| 23:BB:2575:C:H4'   | 26:BD:148:GLN:C   | 2.20                     | 0.66              |
| 35:BN:33:ILE:HD13  | 35:BN:33:ILE:N    | 2.10                     | 0.66              |
| 37:BP:99:LEU:HD12  | 37:BP:101:GLU:OE2 | 1.96                     | 0.66              |
| 40:BS:32:ALA:C     | 40:BS:33:LEU:HD22 | 2.21                     | 0.66              |
| 42:BU:5:ARG:HG2    | 42:BU:6:ARG:H     | 1.60                     | 0.66              |
| 1:CA:205:A:H2'     | 1:CA:206:C:H6     | 1.61                     | 0.66              |
| 1:CA:1053:G:HO2'   | 1:CA:1199:U:H5    | 1.42                     | 0.66              |
| 1:CA:1461:G:H2'    | 1:CA:1462:C:H6    | 1.59                     | 0.66              |
| 2:CC:176:THR:OG1   | 2:CC:179:ALA:HB2  | 1.96                     | 0.66              |
| 5:CF:88:MET:HE3    | 5:CF:90:MET:HG3   | 1.76                     | 0.66              |
| 23:DB:580:U:H2'    | 23:DB:581:C:C6    | 2.29                     | 0.66              |
| 23:DB:928:A:H1'    | 45:DY:1:ALA:HA    | 1.77                     | 0.66              |
| 23:DB:943:A:P      | 33:DL:40:SER:HA   | 2.35                     | 0.66              |
| 23:DB:1099:G:C5'   | 52:DI:3:LYS:N     | 2.59                     | 0.66              |
| 25:DC:75:ALA:HB1   | 25:DC:93:VAL:HG13 | 1.78                     | 0.66              |
| 26:DD:129:THR:HG23 | 26:DD:130:GLN:H   | 1.60                     | 0.66              |
| 36:DO:25:ARG:CG    | 36:DO:94:ARG:HH22 | 2.08                     | 0.66              |
| 42:DU:71:ILE:HD13  | 42:DU:72:PHE:N    | 2.11                     | 0.66              |
| 43:DW:42:THR:HB    | 43:DW:75:ASN:CG   | 2.21                     | 0.66              |
| 45:DY:2:LYS:CB     | 45:DY:37:ARG:HB2  | 2.25                     | 0.66              |
| 1:AA:37:U:P        | 11:AL:119:LYS:HB2 | 2.35                     | 0.66              |
| 1:AA:539:A:H2'     | 1:AA:540:G:C8     | 2.31                     | 0.66              |
| 1:AA:555:U:H2'     | 1:AA:556:C:H6     | 1.60                     | 0.66              |
| 1:AA:731:G:H5'     | 1:AA:766:A:H4'    | 1.78                     | 0.66              |
| 1:AA:1110:A:H2'    | 1:AA:1111:A:H8    | 1.61                     | 0.66              |
| 3:AD:187:ARG:HA    | 3:AD:190:LEU:HD22 | 1.78                     | 0.66              |
| 7:AH:9:MET:HA      | 7:AH:26:MET:HE2   | 1.77                     | 0.66              |
| 23:BB:1456:G:O2'   | 23:BB:1457:U:H5'  | 1.95                     | 0.66              |
| 25:BC:257:ARG:NH1  | 25:BC:257:ARG:HA  | 2.11                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:BM:100:LYS:HE3 | 34:BM:100:LYS:N    | 2.10                     | 0.66              |
| 40:BS:70:LYS:HD2  | 40:BS:110:ARG:HA   | 1.78                     | 0.66              |
| 1:CA:312:C:H2'    | 1:CA:313:A:C8      | 2.31                     | 0.66              |
| 1:CA:1286:U:O2'   | 1:CA:1287:A:H5''   | 1.96                     | 0.66              |
| 9:CJ:41:PRO:HA    | 9:CJ:72:ARG:HD3    | 1.77                     | 0.66              |
| 10:CK:124:LYS:HD3 | 21:CU:34:ARG:HD3   | 1.76                     | 0.66              |
| 20:CB:26:MET:HE1  | 20:CB:186:VAL:HB   | 1.77                     | 0.66              |
| 23:DB:564:C:O2'   | 23:DB:565:C:H5'    | 1.95                     | 0.66              |
| 23:DB:589:U:H2'   | 23:DB:590:A:C8     | 2.30                     | 0.66              |
| 23:DB:1083:U:H1'  | 23:DB:1086:A:H61   | 1.60                     | 0.66              |
| 23:DB:1098:A:C4   | 52:DI:3:LYS:O      | 2.49                     | 0.66              |
| 25:DC:48:ILE:HG22 | 25:DC:49:THR:N     | 2.05                     | 0.66              |
| 25:DC:208:GLY:HA2 | 25:DC:212:TRP:HB3  | 1.78                     | 0.66              |
| 34:DM:16:ARG:HE   | 34:DM:18:ARG:HH12  | 1.42                     | 0.66              |
| 34:DM:71:LYS:NZ   | 34:DM:91:TYR:HB3   | 2.10                     | 0.66              |
| 34:DM:92:TRP:CD1  | 34:DM:93:VAL:H     | 2.13                     | 0.66              |
| 43:DW:30:VAL:HG12 | 43:DW:31:LEU:H     | 1.61                     | 0.66              |
| 43:DW:44:PHE:HB3  | 43:DW:77:LYS:HB3   | 1.76                     | 0.66              |
| 46:DZ:30:HIS:CE1  | 46:DZ:49:ARG:HH12  | 2.14                     | 0.66              |
| 52:DI:41:PHE:O    | 52:DI:45:THR:HG23  | 1.96                     | 0.66              |
| 1:AA:16:A:O2'     | 1:AA:17:U:H5'      | 1.95                     | 0.66              |
| 1:AA:239:U:H6     | 1:AA:239:U:C5'     | 2.08                     | 0.66              |
| 3:AD:56:GLU:HG2   | 3:AD:195:ASN:HD22  | 1.60                     | 0.66              |
| 23:BB:1219:U:H2'  | 23:BB:1220:G:C8    | 2.30                     | 0.66              |
| 26:BD:35:THR:HB   | 26:BD:48:ILE:HB    | 1.76                     | 0.66              |
| 28:BF:34:THR:HG23 | 28:BF:89:THR:HG22  | 1.76                     | 0.66              |
| 33:BL:62:PRO:C    | 50:B3:24:LYS:HD3   | 2.20                     | 0.66              |
| 33:BL:78:ARG:HD3  | 33:BL:81:ASP:HB2   | 1.78                     | 0.66              |
| 34:BM:22:GLN:HG2  | 34:BM:23:GLY:N     | 2.11                     | 0.66              |
| 44:BX:49:ASP:HB3  | 44:BX:52:ARG:HH21  | 1.59                     | 0.66              |
| 48:B1:15:GLY:H    | 48:B1:47:ILE:HD12  | 1.60                     | 0.66              |
| 1:CA:539:A:H2'    | 1:CA:540:G:C8      | 2.30                     | 0.66              |
| 1:CA:586:C:O2'    | 1:CA:587:G:H5'     | 1.95                     | 0.66              |
| 1:CA:1024:G:O2'   | 1:CA:1025:U:H5'    | 1.94                     | 0.66              |
| 1:CA:1513:A:H2'   | 1:CA:1514:G:H8     | 1.60                     | 0.66              |
| 5:CF:47:LEU:HD21  | 5:CF:57:ALA:HB2    | 1.77                     | 0.66              |
| 12:CM:73:SER:HB3  | 12:CM:77:LYS:HE2   | 1.77                     | 0.66              |
| 18:CS:28:LYS:HB3  | 18:CS:28:LYS:HZ2   | 1.60                     | 0.66              |
| 20:CB:137:THR:HA  | 20:CB:140:LEU:HD12 | 1.77                     | 0.66              |
| 22:DA:47:C:H5'    | 36:DO:97:PHE:CZ    | 2.31                     | 0.66              |
| 23:DB:65:U:H2'    | 23:DB:66:C:H6      | 1.61                     | 0.66              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DB:143:C:H6     | 23:DB:143:C:O5'   | 1.79                     | 0.66              |
| 23:DB:235:U:H2'    | 23:DB:236:C:C6    | 2.30                     | 0.66              |
| 23:DB:289:G:H2'    | 23:DB:290:U:H6    | 1.58                     | 0.66              |
| 23:DB:414:C:H2'    | 23:DB:415:A:H8    | 1.59                     | 0.66              |
| 23:DB:2591:C:H2'   | 23:DB:2592:G:C8   | 2.31                     | 0.66              |
| 39:DR:41:ILE:HG13  | 39:DR:43:ASN:HD22 | 1.61                     | 0.66              |
| 40:DS:84:ARG:HH21  | 40:DS:98:LYS:NZ   | 1.94                     | 0.66              |
| 43:DW:42:THR:H     | 43:DW:65:LYS:HA   | 1.61                     | 0.66              |
| 1:AA:1300:G:H1'    | 1:AA:1301:U:C5    | 2.31                     | 0.66              |
| 23:BB:142:A:H2'    | 23:BB:143:C:C6    | 2.31                     | 0.66              |
| 23:BB:2246:G:H2'   | 23:BB:2247:A:C8   | 2.30                     | 0.66              |
| 23:BB:2461:A:H2'   | 23:BB:2462:C:H6   | 1.59                     | 0.66              |
| 29:BG:86:LEU:HB2   | 29:BG:130:ILE:HB  | 1.76                     | 0.66              |
| 31:BJ:24:THR:HB    | 31:BJ:27:ARG:HB2  | 1.78                     | 0.66              |
| 35:BN:28:LEU:HD12  | 35:BN:28:LEU:H    | 1.61                     | 0.66              |
| 38:BQ:95:ALA:C     | 38:BQ:97:ILE:H    | 2.03                     | 0.66              |
| 52:BI:91:LYS:HB2   | 52:BI:94:LYS:HD2  | 1.78                     | 0.66              |
| 1:CA:997:U:H2'     | 1:CA:998:C:C6     | 2.30                     | 0.66              |
| 1:CA:1462:C:H4'    | 37:DP:110:LYS:HE2 | 1.77                     | 0.66              |
| 6:CG:42:VAL:O      | 6:CG:46:LEU:HB2   | 1.96                     | 0.66              |
| 10:CK:12:ARG:N     | 10:CK:76:TYR:HA   | 2.10                     | 0.66              |
| 12:CM:78:ARG:O     | 12:CM:82:LEU:HG   | 1.95                     | 0.66              |
| 23:DB:304:U:H2'    | 23:DB:305:C:C6    | 2.31                     | 0.66              |
| 44:DX:11:VAL:HG12  | 44:DX:13:GLU:H    | 1.60                     | 0.66              |
| 1:AA:56:U:H2'      | 1:AA:57:G:H8      | 1.61                     | 0.66              |
| 2:AC:154:GLY:HA3   | 2:AC:162:ALA:HB1  | 1.75                     | 0.66              |
| 7:AH:55:LYS:HA     | 7:AH:55:LYS:HE3   | 1.77                     | 0.66              |
| 9:AJ:6:ILE:HA      | 9:AJ:102:LEU:HG   | 1.78                     | 0.66              |
| 11:AL:42:LYS:HE3   | 11:AL:90:PRO:HD3  | 1.78                     | 0.66              |
| 11:AL:106:VAL:HG22 | 11:AL:116:TYR:HB3 | 1.76                     | 0.66              |
| 23:BB:564:C:O2'    | 23:BB:565:C:H5'   | 1.95                     | 0.66              |
| 23:BB:594:U:H2'    | 23:BB:595:C:H6    | 1.60                     | 0.66              |
| 23:BB:1060:U:OP2   | 52:BI:74:PRO:HA   | 1.95                     | 0.66              |
| 23:BB:1645:G:H5''  | 23:BB:1646:C:H5'  | 1.78                     | 0.66              |
| 25:BC:204:LEU:HB3  | 25:BC:210:ALA:HB1 | 1.78                     | 0.66              |
| 26:BD:21:SER:C     | 26:BD:23:PRO:HD3  | 2.20                     | 0.66              |
| 26:BD:170:VAL:HG13 | 26:BD:171:THR:N   | 2.08                     | 0.66              |
| 28:BF:125:GLY:HA3  | 28:BF:159:ALA:HB3 | 1.77                     | 0.66              |
| 30:BH:26:ALA:HA    | 30:BH:30:LEU:HB2  | 1.77                     | 0.66              |
| 31:BJ:119:PHE:CG   | 31:BJ:120:ARG:N   | 2.61                     | 0.66              |
| 33:BL:142:ILE:HG13 | 33:BL:143:GLU:N   | 2.10                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:BP:38:ARG:HG3   | 37:BP:39:LEU:H     | 1.61                     | 0.66              |
| 39:BR:23:GLU:HA    | 39:BR:96:VAL:HG13  | 1.77                     | 0.66              |
| 41:BT:24:MET:HE2   | 41:BT:29:THR:H     | 1.61                     | 0.66              |
| 1:CA:105:G:H2'     | 1:CA:106:C:C6      | 2.31                     | 0.66              |
| 1:CA:960:U:O2'     | 1:CA:1223:C:H5'    | 1.96                     | 0.66              |
| 1:CA:1132:C:H2'    | 1:CA:1133:G:C8     | 2.30                     | 0.66              |
| 1:CA:1422:G:O2'    | 1:CA:1423:G:H5'    | 1.95                     | 0.66              |
| 2:CC:61:LYS:HZ3    | 2:CC:96:VAL:HG12   | 1.60                     | 0.66              |
| 4:CE:81:GLN:HE22   | 4:CE:148:SER:HA    | 1.61                     | 0.66              |
| 5:CF:35:LYS:O      | 5:CF:64:VAL:HG13   | 1.95                     | 0.66              |
| 8:CI:14:SER:HA     | 8:CI:68:GLY:O      | 1.96                     | 0.66              |
| 16:CQ:45:VAL:HG21  | 16:CQ:60:ILE:HG21  | 1.77                     | 0.66              |
| 23:DB:728:G:H1'    | 25:DC:16:VAL:HG21  | 1.77                     | 0.66              |
| 23:DB:813:U:H2'    | 23:DB:814:C:C6     | 2.31                     | 0.66              |
| 24:DV:53:LYS:HZ2   | 24:DV:55:GLU:HG2   | 1.60                     | 0.66              |
| 31:DJ:97:PRO:O     | 31:DJ:100:VAL:HG12 | 1.96                     | 0.66              |
| 37:DP:71:ARG:O     | 37:DP:72:VAL:HG22  | 1.96                     | 0.66              |
| 42:DU:22:GLY:HA3   | 42:DU:35:VAL:HG23  | 1.78                     | 0.66              |
| 46:DZ:27:THR:O     | 46:DZ:28:VAL:HG13  | 1.96                     | 0.66              |
| 5:AF:86:ARG:NH1    | 17:AR:63:TYR:HB3   | 2.11                     | 0.65              |
| 13:AN:30:ILE:HB    | 13:AN:44:VAL:HG11  | 1.78                     | 0.65              |
| 23:BB:691:C:H4'    | 25:BC:42:ARG:NE    | 2.11                     | 0.65              |
| 23:BB:704:G:H1'    | 23:BB:727:A:H61    | 1.60                     | 0.65              |
| 23:BB:857:G:C2'    | 23:BB:858:G:H5'    | 2.26                     | 0.65              |
| 23:BB:869:G:H2'    | 23:BB:870:U:H6     | 1.61                     | 0.65              |
| 23:BB:2049:G:O2'   | 23:BB:2050:C:H5'   | 1.96                     | 0.65              |
| 23:BB:2758:A:H2'   | 23:BB:2759:G:O4'   | 1.96                     | 0.65              |
| 26:BD:167:ASN:HD22 | 26:BD:167:ASN:H    | 1.43                     | 0.65              |
| 38:BQ:85:ALA:CB    | 38:BQ:88:GLU:HB2   | 2.26                     | 0.65              |
| 41:BT:77:ARG:HG2   | 41:BT:78:SER:H     | 1.60                     | 0.65              |
| 1:CA:376:G:H4'     | 15:CP:5:ARG:HD3    | 1.78                     | 0.65              |
| 1:CA:1119:C:H2'    | 1:CA:1120:C:H6     | 1.60                     | 0.65              |
| 2:CC:166:TRP:CG    | 2:CC:167:TYR:N     | 2.65                     | 0.65              |
| 4:CE:82:HIS:CE1    | 7:CH:95:MET:HE2    | 2.32                     | 0.65              |
| 4:CE:131:ASN:O     | 4:CE:135:VAL:HG23  | 1.95                     | 0.65              |
| 13:CN:11:LYS:O     | 13:CN:15:LEU:HG    | 1.96                     | 0.65              |
| 23:DB:2295:C:O2'   | 23:DB:2296:U:H5'   | 1.96                     | 0.65              |
| 24:DV:2:PHE:HB2    | 24:DV:61:LEU:HD22  | 1.78                     | 0.65              |
| 25:DC:20:ASN:HB2   | 25:DC:202:ARG:HD3  | 1.78                     | 0.65              |
| 25:DC:161:VAL:HG12 | 25:DC:173:LEU:HD22 | 1.77                     | 0.65              |
| 31:DJ:18:VAL:O     | 31:DJ:56:VAL:HA    | 1.96                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:DM:55:ARG:O     | 34:DM:57:VAL:HG23  | 1.96                     | 0.65              |
| 35:DN:45:ARG:CZ    | 35:DN:95:THR:HB    | 2.26                     | 0.65              |
| 35:DN:45:ARG:NH2   | 35:DN:113:ILE:HG23 | 2.04                     | 0.65              |
| 44:DX:31:GLN:HA    | 44:DX:31:GLN:HE21  | 1.59                     | 0.65              |
| 51:D4:2:LYS:HB2    | 51:D4:2:LYS:NZ     | 2.10                     | 0.65              |
| 1:AA:105:G:H2'     | 1:AA:106:C:C6      | 2.31                     | 0.65              |
| 1:AA:312:C:H2'     | 1:AA:313:A:C8      | 2.30                     | 0.65              |
| 9:AJ:37:ARG:NE     | 9:AJ:77:VAL:HG11   | 2.12                     | 0.65              |
| 21:AU:39:LYS:N     | 21:AU:40:PRO:HD2   | 2.10                     | 0.65              |
| 23:BB:6:A:H2'      | 23:BB:7:G:H8       | 1.62                     | 0.65              |
| 23:BB:1076:C:H4'   | 52:BI:94:LYS:NZ    | 2.11                     | 0.65              |
| 23:BB:1533:C:O2'   | 23:BB:1534:U:H5'   | 1.95                     | 0.65              |
| 23:BB:2027:G:O2'   | 23:BB:2028:U:H5'   | 1.96                     | 0.65              |
| 34:BM:17:ASN:C     | 34:BM:18:ARG:HD3   | 2.22                     | 0.65              |
| 35:BN:49:GLU:HB2   | 35:BN:50:PRO:HD3   | 1.77                     | 0.65              |
| 45:BY:6:ILE:H      | 45:BY:6:ILE:HD13   | 1.61                     | 0.65              |
| 1:CA:37:U:OP1      | 11:CL:120:ARG:HB3  | 1.96                     | 0.65              |
| 1:CA:501:C:H2'     | 1:CA:502:A:C8      | 2.31                     | 0.65              |
| 1:CA:1060:U:H2'    | 1:CA:1061:G:H8     | 1.61                     | 0.65              |
| 1:CA:1320:C:OP1    | 18:CS:69:LYS:HE3   | 1.96                     | 0.65              |
| 4:CE:87:VAL:HG13   | 4:CE:88:HIS:N      | 2.10                     | 0.65              |
| 23:DB:2012:G:H4'   | 40:DS:96:ILE:HD11  | 1.78                     | 0.65              |
| 23:DB:2443:C:H2'   | 23:DB:2444:G:C8    | 2.31                     | 0.65              |
| 26:DD:146:ILE:HG12 | 26:DD:155:VAL:HG13 | 1.76                     | 0.65              |
| 39:DR:74:ILE:HG13  | 39:DR:76:LYS:HG3   | 1.78                     | 0.65              |
| 43:DW:19:ARG:NH1   | 43:DW:19:ARG:HB2   | 2.11                     | 0.65              |
| 1:AA:93:U:H3'      | 1:AA:94:G:H5'      | 1.78                     | 0.65              |
| 23:BB:1590:A:H2'   | 23:BB:1591:A:C8    | 2.32                     | 0.65              |
| 25:BC:21:PRO:O     | 25:BC:22:GLU:HB2   | 1.96                     | 0.65              |
| 25:BC:139:THR:HA   | 25:BC:193:GLU:OE1  | 1.96                     | 0.65              |
| 25:BC:253:GLY:C    | 25:BC:254:LYS:HD2  | 2.21                     | 0.65              |
| 26:BD:128:ARG:HH22 | 26:BD:130:GLN:CD   | 2.05                     | 0.65              |
| 43:BW:44:PHE:O     | 43:BW:75:ASN:HB3   | 1.96                     | 0.65              |
| 44:BX:9:LYS:HE3    | 44:BX:11:VAL:HG13  | 1.78                     | 0.65              |
| 1:CA:389:A:H3'     | 1:CA:390:U:H6      | 1.61                     | 0.65              |
| 1:CA:518:C:H2'     | 1:CA:530:G:C8      | 2.31                     | 0.65              |
| 10:CK:88:PRO:CD    | 21:CU:28:LEU:HD13  | 2.26                     | 0.65              |
| 20:CB:208:ALA:O    | 20:CB:211:LEU:HB3  | 1.96                     | 0.65              |
| 23:DB:181:A:H1'    | 23:DB:435:C:H5'    | 1.78                     | 0.65              |
| 23:DB:899:A:H3'    | 23:DB:900:A:C8     | 2.30                     | 0.65              |
| 23:DB:1098:A:C3'   | 52:DI:3:LYS:C      | 2.69                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:1197:G:H2'   | 23:DB:1198:U:H6    | 1.62                     | 0.65              |
| 23:DB:1381:G:C2'   | 23:DB:1382:G:H5'   | 2.26                     | 0.65              |
| 23:DB:1590:A:H2'   | 23:DB:1591:A:C8    | 2.32                     | 0.65              |
| 23:DB:2027:G:O2'   | 23:DB:2028:U:H5'   | 1.96                     | 0.65              |
| 23:DB:2307:G:H2'   | 23:DB:2307:G:N3    | 2.11                     | 0.65              |
| 26:DD:46:ARG:HA    | 26:DD:82:PHE:HA    | 1.79                     | 0.65              |
| 26:DD:146:ILE:N    | 26:DD:146:ILE:HD12 | 2.11                     | 0.65              |
| 26:DD:151:THR:O    | 26:DD:153:GLY:N    | 2.28                     | 0.65              |
| 34:DM:40:ARG:HA    | 34:DM:92:TRP:HE1   | 1.62                     | 0.65              |
| 37:DP:50:ARG:HH12  | 37:DP:62:LYS:HB2   | 1.59                     | 0.65              |
| 38:DQ:88:GLU:CD    | 39:DR:53:PHE:HB2   | 2.21                     | 0.65              |
| 46:DZ:5:ILE:O      | 46:DZ:51:VAL:HG13  | 1.96                     | 0.65              |
| 52:DI:1:ALA:C      | 52:DI:2:LYS:HD2    | 2.21                     | 0.65              |
| 1:AA:1381:U:O2'    | 1:AA:1382:C:H5'    | 1.97                     | 0.65              |
| 2:AC:141:MET:HE1   | 2:AC:147:GLY:H     | 1.61                     | 0.65              |
| 11:AL:37:TYR:HB2   | 11:AL:51:VAL:HG23  | 1.79                     | 0.65              |
| 20:AB:52:ALA:O     | 20:AB:56:LEU:HD13  | 1.96                     | 0.65              |
| 23:BB:95:A:H4'     | 44:BX:40:SER:HB3   | 1.78                     | 0.65              |
| 23:BB:710:U:H2'    | 23:BB:711:G:H8     | 1.61                     | 0.65              |
| 23:BB:936:A:H2'    | 23:BB:937:C:C6     | 2.30                     | 0.65              |
| 23:BB:1112:G:H4'   | 29:BG:2:ARG:HG2    | 1.78                     | 0.65              |
| 23:BB:2008:C:H2'   | 23:BB:2009:A:C8    | 2.31                     | 0.65              |
| 24:BV:76:ASP:HB2   | 34:BM:136:MET:HG3  | 1.78                     | 0.65              |
| 25:BC:10:PRO:HD2   | 25:BC:202:ARG:NH1  | 2.11                     | 0.65              |
| 26:BD:92:VAL:HG22  | 26:BD:94:GLN:HB2   | 1.78                     | 0.65              |
| 27:BE:130:LYS:HE2  | 27:BE:130:LYS:HA   | 1.77                     | 0.65              |
| 28:BF:110:ILE:HG22 | 28:BF:112:ASP:H    | 1.61                     | 0.65              |
| 28:BF:135:ILE:C    | 28:BF:137:PHE:H    | 2.04                     | 0.65              |
| 42:BU:7:ASP:CA     | 42:BU:24:VAL:HA    | 2.26                     | 0.65              |
| 44:BX:5:GLU:H      | 44:BX:7:ARG:HE     | 1.44                     | 0.65              |
| 47:B0:2:VAL:HG22   | 47:B0:3:GLN:N      | 2.11                     | 0.65              |
| 1:CA:1343:G:H2'    | 1:CA:1344:C:C6     | 2.31                     | 0.65              |
| 8:CI:94:ARG:HD3    | 8:CI:97:LEU:HD12   | 1.79                     | 0.65              |
| 13:CN:31:SER:HA    | 13:CN:40:ARG:HA    | 1.77                     | 0.65              |
| 23:DB:4:U:H2'      | 23:DB:5:A:C8       | 2.31                     | 0.65              |
| 23:DB:225:C:O2'    | 23:DB:226:A:H5'    | 1.97                     | 0.65              |
| 23:DB:1714:U:H3'   | 23:DB:1715:G:H5'   | 1.77                     | 0.65              |
| 23:DB:2461:A:H2'   | 23:DB:2462:C:H6    | 1.60                     | 0.65              |
| 25:DC:32:LEU:HA    | 25:DC:81:GLU:OE2   | 1.96                     | 0.65              |
| 25:DC:137:GLY:C    | 25:DC:139:THR:H    | 2.02                     | 0.65              |
| 26:DD:122:VAL:HG21 | 26:DD:141:ARG:HD3  | 1.78                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:DG:39:ALA:O     | 29:DG:41:GLU:HG3   | 1.96                     | 0.65              |
| 33:DL:63:LYS:HB2   | 50:D3:26:ALA:HB2   | 1.78                     | 0.65              |
| 38:DQ:9:ALA:O      | 38:DQ:12:ARG:HB3   | 1.97                     | 0.65              |
| 40:DS:82:MET:HE3   | 40:DS:84:ARG:HB2   | 1.78                     | 0.65              |
| 42:DU:59:GLU:HG2   | 42:DU:60:LYS:N     | 2.10                     | 0.65              |
| 47:D0:27:LEU:HD22  | 47:D0:27:LEU:N     | 2.11                     | 0.65              |
| 47:D0:41:HIS:HB3   | 47:D0:47:TYR:H     | 1.62                     | 0.65              |
| 1:AA:967:C:OP1     | 1:AA:969:A:H5'     | 1.97                     | 0.65              |
| 2:AC:88:LYS:O      | 2:AC:88:LYS:HD3    | 1.97                     | 0.65              |
| 13:AN:12:ARG:HH11  | 13:AN:60:ARG:NH1   | 1.94                     | 0.65              |
| 15:AP:42:ILE:HG22  | 15:AP:43:ALA:N     | 2.12                     | 0.65              |
| 23:BB:1856:U:H2'   | 23:BB:1857:G:O4'   | 1.96                     | 0.65              |
| 23:BB:2591:C:H2'   | 23:BB:2592:G:C8    | 2.31                     | 0.65              |
| 37:BP:52:ARG:HG2   | 37:BP:54:LEU:HB2   | 1.77                     | 0.65              |
| 38:BQ:47:ARG:O     | 38:BQ:51:GLN:HB3   | 1.97                     | 0.65              |
| 40:BS:17:VAL:HA    | 40:BS:43:ALA:HB1   | 1.77                     | 0.65              |
| 42:BU:44:HIS:HB2   | 42:BU:56:GLY:N     | 2.11                     | 0.65              |
| 1:CA:190:A:O5'     | 1:CA:190:A:H8      | 1.80                     | 0.65              |
| 1:CA:1132:C:H2'    | 1:CA:1133:G:H8     | 1.61                     | 0.65              |
| 12:CM:48:SER:H     | 12:CM:51:GLN:HE22  | 1.43                     | 0.65              |
| 20:CB:153:MET:SD   | 20:CB:157:PRO:HD3  | 2.35                     | 0.65              |
| 22:DA:5:U:H2'      | 22:DA:6:G:H8       | 1.61                     | 0.65              |
| 23:DB:1098:A:C2'   | 52:DI:3:LYS:C      | 2.70                     | 0.65              |
| 23:DB:1360:G:H2'   | 23:DB:1361:G:H5'   | 1.79                     | 0.65              |
| 23:DB:1645:G:H5''  | 23:DB:1646:C:H5'   | 1.78                     | 0.65              |
| 27:DE:1:MET:HG3    | 27:DE:18:THR:OG1   | 1.96                     | 0.65              |
| 29:DG:169:ARG:NH1  | 29:DG:169:ARG:HB2  | 2.10                     | 0.65              |
| 36:DO:4:LYS:HD2    | 36:DO:5:SER:N      | 2.12                     | 0.65              |
| 50:D3:49:VAL:HG22  | 50:D3:50:SER:N     | 2.08                     | 0.65              |
| 52:DI:108:ILE:HG22 | 52:DI:128:ILE:HD13 | 1.79                     | 0.65              |
| 1:AA:1118:U:H1'    | 1:AA:1179:A:C4     | 2.31                     | 0.65              |
| 2:AC:19:SER:HB2    | 2:AC:39:ARG:HH22   | 1.61                     | 0.65              |
| 2:AC:72:PRO:O      | 2:AC:76:ILE:HG12   | 1.95                     | 0.65              |
| 14:AO:81:ILE:HA    | 14:AO:86:LEU:HD12  | 1.78                     | 0.65              |
| 20:AB:112:ARG:O    | 20:AB:116:LEU:HB2  | 1.96                     | 0.65              |
| 23:BB:423:A:H5'    | 23:BB:424:G:C5'    | 2.26                     | 0.65              |
| 23:BB:1155:A:H61   | 45:BY:10:ARG:NH1   | 1.94                     | 0.65              |
| 23:BB:2133:G:H2'   | 23:BB:2133:G:N3    | 2.10                     | 0.65              |
| 23:BB:2204:G:C5'   | 25:BC:149:LYS:HE3  | 2.21                     | 0.65              |
| 23:BB:2784:U:H5''  | 26:BD:41:ALA:HB1   | 1.79                     | 0.65              |
| 23:BB:2876:G:H4'   | 37:BP:2:ASN:HA     | 1.77                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BE:190:ALA:HB1  | 27:BE:193:VAL:HB   | 1.79                     | 0.65              |
| 36:BO:98:GLN:O     | 36:BO:103:VAL:HG21 | 1.97                     | 0.65              |
| 41:BT:64:LYS:HB3   | 41:BT:77:ARG:HH11  | 1.60                     | 0.65              |
| 1:CA:163:C:H2'     | 1:CA:164:G:O4'     | 1.97                     | 0.65              |
| 5:CF:39:LEU:HD22   | 5:CF:39:LEU:O      | 1.97                     | 0.65              |
| 23:DB:25:U:H5''    | 40:DS:80:PRO:HD3   | 1.78                     | 0.65              |
| 23:DB:587:C:C3'    | 33:DL:29:LYS:HD2   | 2.13                     | 0.65              |
| 23:DB:1856:U:H2'   | 23:DB:1857:G:O4'   | 1.96                     | 0.65              |
| 33:DL:59:ARG:NH1   | 50:D3:58:ILE:HG21  | 2.12                     | 0.65              |
| 36:DO:25:ARG:HE    | 36:DO:94:ARG:NH1   | 1.94                     | 0.65              |
| 47:D0:47:TYR:HB3   | 47:D0:52:LYS:N     | 2.11                     | 0.65              |
| 52:DI:32:VAL:HG22  | 52:DI:60:VAL:HG21  | 1.78                     | 0.65              |
| 1:AA:312:C:H2'     | 1:AA:313:A:H8      | 1.62                     | 0.65              |
| 1:AA:1171:A:H2'    | 1:AA:1172:C:H6     | 1.62                     | 0.65              |
| 5:AF:17:GLN:HG2    | 5:AF:21:MET:HG3    | 1.78                     | 0.65              |
| 14:AO:70:LYS:HZ3   | 14:AO:74:VAL:HG13  | 1.62                     | 0.65              |
| 20:AB:185:ILE:HA   | 20:AB:199:ILE:HB   | 1.78                     | 0.65              |
| 20:AB:204:ASP:CG   | 20:AB:205:ALA:H    | 2.03                     | 0.65              |
| 23:BB:813:U:H2'    | 23:BB:814:C:C6     | 2.32                     | 0.65              |
| 23:BB:958:U:C4     | 34:BM:18:ARG:HB2   | 2.31                     | 0.65              |
| 23:BB:1901:A:H1'   | 25:BC:250:GLN:HE22 | 1.60                     | 0.65              |
| 27:BE:128:ALA:HA   | 27:BE:157:LEU:HD22 | 1.79                     | 0.65              |
| 28:BF:107:VAL:N    | 28:BF:108:PRO:HD2  | 2.12                     | 0.65              |
| 31:BJ:58:ASN:HA    | 31:BJ:126:ALA:HA   | 1.78                     | 0.65              |
| 33:BL:63:LYS:HG2   | 50:B3:11:LYS:HA    | 1.77                     | 0.65              |
| 39:BR:75:VAL:H     | 39:BR:90:ARG:HE    | 1.43                     | 0.65              |
| 1:CA:882:C:O2'     | 1:CA:883:C:H5'     | 1.96                     | 0.65              |
| 1:CA:1527:U:H2'    | 1:CA:1528:U:C6     | 2.31                     | 0.65              |
| 9:CJ:56:HIS:O      | 9:CJ:57:VAL:HG12   | 1.96                     | 0.65              |
| 10:CK:115:ILE:O    | 10:CK:115:ILE:HD12 | 1.96                     | 0.65              |
| 16:CQ:10:ARG:NH2   | 16:CQ:11:VAL:HB    | 2.11                     | 0.65              |
| 23:DB:179:C:H5''   | 49:D2:28:ARG:HH12  | 1.60                     | 0.65              |
| 23:DB:222:A:N6     | 23:DB:232:G:H1'    | 2.12                     | 0.65              |
| 25:DC:171:VAL:HA   | 25:DC:183:VAL:O    | 1.97                     | 0.65              |
| 28:DF:83:PRO:O     | 28:DF:84:ILE:HD12  | 1.96                     | 0.65              |
| 29:DG:53:PRO:HG2   | 29:DG:61:TRP:CZ3   | 2.32                     | 0.65              |
| 32:DK:99:ILE:HD13  | 32:DK:115:ILE:HG13 | 1.78                     | 0.65              |
| 35:DN:42:LYS:HE3   | 35:DN:42:LYS:HA    | 1.78                     | 0.65              |
| 35:DN:107:ASN:HD22 | 40:DS:40:ASN:HD22  | 1.43                     | 0.65              |
| 41:DT:48:GLN:CA    | 41:DT:53:VAL:HG22  | 2.25                     | 0.65              |
| 1:AA:163:C:H2'     | 1:AA:164:G:O4'     | 1.97                     | 0.65              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:882:C:O2'    | 1:AA:883:C:H5'    | 1.96                     | 0.65              |
| 1:AA:1471:U:O2'   | 1:AA:1472:U:H5'   | 1.97                     | 0.65              |
| 10:AK:30:ILE:HG22 | 10:AK:45:THR:HA   | 1.79                     | 0.65              |
| 12:AM:44:ILE:HA   | 12:AM:47:LEU:HD13 | 1.79                     | 0.65              |
| 19:AT:68:LYS:CG   | 19:AT:69:ASN:H    | 2.05                     | 0.65              |
| 23:BB:161:A:C3'   | 23:BB:162:U:H5''  | 2.19                     | 0.65              |
| 23:BB:1979:U:O2'  | 23:BB:1980:G:H5'  | 1.96                     | 0.65              |
| 27:BE:84:THR:HG23 | 27:BE:85:PHE:H    | 1.61                     | 0.65              |
| 33:BL:77:ILE:HB   | 33:BL:110:VAL:CG2 | 2.26                     | 0.65              |
| 49:B2:25:LYS:HE3  | 49:B2:25:LYS:N    | 2.10                     | 0.65              |
| 52:BI:121:ILE:HA  | 52:BI:124:MET:HE3 | 1.77                     | 0.65              |
| 1:CA:372:C:H1'    | 1:CA:373:A:OP2    | 1.97                     | 0.65              |
| 1:CA:1069:C:H4'   | 1:CA:1192:C:O2    | 1.97                     | 0.65              |
| 1:CA:1191:A:OP1   | 2:CC:3:LYS:HG3    | 1.97                     | 0.65              |
| 1:CA:1380:U:O4    | 6:CG:2:ARG:HB2    | 1.97                     | 0.65              |
| 1:CA:1386:G:H2'   | 1:CA:1387:G:H8    | 1.61                     | 0.65              |
| 3:CD:141:VAL:HG12 | 3:CD:180:THR:HA   | 1.77                     | 0.65              |
| 5:CF:53:LYS:HD3   | 5:CF:54:LEU:HB2   | 1.79                     | 0.65              |
| 6:CG:15:PRO:HG2   | 6:CG:43:TYR:OH    | 1.96                     | 0.65              |
| 8:CI:33:SER:H     | 8:CI:36:GLN:HB2   | 1.61                     | 0.65              |
| 22:DA:5:U:H2'     | 22:DA:6:G:C8      | 2.32                     | 0.65              |
| 23:DB:139:U:H3'   | 23:DB:139:U:P     | 2.37                     | 0.65              |
| 23:DB:1105:U:H2'  | 23:DB:1106:G:H8   | 1.60                     | 0.65              |
| 23:DB:1262:A:H2   | 47:D0:6:LYS:HD2   | 1.62                     | 0.65              |
| 23:DB:1515:A:H2'  | 23:DB:1516:G:O4'  | 1.97                     | 0.65              |
| 23:DB:2537:U:H2'  | 23:DB:2538:C:H6   | 1.60                     | 0.65              |
| 26:DD:1:MET:HB2   | 26:DD:81:GLU:OE1  | 1.97                     | 0.65              |
| 26:DD:48:ILE:HG22 | 26:DD:49:GLN:N    | 2.12                     | 0.65              |
| 30:DH:53:GLU:OE1  | 30:DH:57:LYS:HD2  | 1.96                     | 0.65              |
| 33:DL:77:ILE:HB   | 33:DL:110:VAL:HA  | 1.77                     | 0.65              |
| 35:DN:73:ASN:O    | 35:DN:76:VAL:HG12 | 1.96                     | 0.65              |
| 39:DR:6:GLN:NE2   | 39:DR:41:ILE:HB   | 2.12                     | 0.65              |
| 23:BB:277:G:H5''  | 23:BB:278:A:N7    | 2.12                     | 0.65              |
| 23:BB:416:U:H2'   | 23:BB:417:C:C6    | 2.31                     | 0.65              |
| 25:BC:117:SER:HB3 | 25:BC:127:ASN:ND2 | 2.12                     | 0.65              |
| 29:BG:157:LYS:HB2 | 29:BG:159:LYS:HG2 | 1.78                     | 0.65              |
| 31:BJ:17:VAL:HG23 | 31:BJ:139:VAL:HB  | 1.79                     | 0.65              |
| 38:BQ:16:ILE:HD13 | 38:BQ:34:ALA:HB2  | 1.77                     | 0.65              |
| 43:BW:57:THR:O    | 43:BW:58:LEU:HB3  | 1.96                     | 0.65              |
| 46:BZ:32:LEU:HD11 | 46:BZ:47:LYS:HG3  | 1.78                     | 0.65              |
| 1:CA:1036:A:H2'   | 1:CA:1037:C:C6    | 2.31                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1270:G:H2'    | 1:CA:1271:A:C8     | 2.32                     | 0.65              |
| 4:CE:87:VAL:HG13   | 4:CE:88:HIS:H      | 1.61                     | 0.65              |
| 6:CG:63:VAL:HG12   | 6:CG:126:ALA:HB1   | 1.78                     | 0.65              |
| 13:CN:25:GLU:O     | 13:CN:29:ILE:HG13  | 1.97                     | 0.65              |
| 23:DB:1368:G:H5''  | 49:D2:25:LYS:CG    | 2.23                     | 0.65              |
| 23:DB:2285:C:C5    | 48:D1:7:LYS:HE3    | 2.32                     | 0.65              |
| 25:DC:170:TYR:O    | 25:DC:171:VAL:HG13 | 1.96                     | 0.65              |
| 26:DD:33:ARG:O     | 26:DD:34:VAL:HG22  | 1.96                     | 0.65              |
| 27:DE:149:ILE:HD11 | 27:DE:188:MET:N    | 2.12                     | 0.65              |
| 28:DF:7:TYR:O      | 28:DF:12:VAL:HG23  | 1.97                     | 0.65              |
| 29:DG:10:VAL:HA    | 29:DG:14:VAL:HG11  | 1.77                     | 0.65              |
| 34:DM:71:LYS:HZ3   | 34:DM:91:TYR:HB3   | 1.61                     | 0.65              |
| 35:DN:38:LEU:HB3   | 35:DN:39:PRO:HD3   | 1.78                     | 0.65              |
| 42:DU:11:ILE:HG22  | 42:DU:12:VAL:H     | 1.61                     | 0.65              |
| 47:D0:29:VAL:HB    | 47:D0:34:GLY:HA2   | 1.77                     | 0.65              |
| 1:AA:1295:U:H2'    | 1:AA:1296:C:C6     | 2.32                     | 0.65              |
| 10:AK:22:ILE:HD13  | 10:AK:95:THR:CG2   | 2.27                     | 0.65              |
| 13:AN:27:LYS:HE2   | 13:AN:48:GLN:HE22  | 1.62                     | 0.65              |
| 20:AB:141:GLU:O    | 20:AB:145:ASN:HB2  | 1.97                     | 0.65              |
| 30:BH:3:VAL:HB     | 30:BH:37:VAL:CB    | 2.26                     | 0.65              |
| 37:BP:38:ARG:HA    | 37:BP:38:ARG:HH11  | 1.62                     | 0.65              |
| 39:BR:24:LYS:HD3   | 39:BR:66:HIS:NE2   | 2.12                     | 0.65              |
| 39:BR:65:ALA:HB3   | 39:BR:99:THR:H     | 1.61                     | 0.65              |
| 4:CE:109:ALA:HB1   | 4:CE:136:VAL:HG13  | 1.77                     | 0.65              |
| 7:CH:11:THR:HA     | 7:CH:14:ARG:NH1    | 2.11                     | 0.65              |
| 23:DB:4:U:H2'      | 23:DB:5:A:H8       | 1.60                     | 0.65              |
| 23:DB:144:A:C2     | 41:DT:3:ARG:NH2    | 2.65                     | 0.65              |
| 23:DB:224:U:O4     | 23:DB:420:C:H5'    | 1.97                     | 0.65              |
| 23:DB:936:A:H2'    | 23:DB:937:C:C6     | 2.32                     | 0.65              |
| 23:DB:1179:G:H2'   | 23:DB:1180:U:H6    | 1.62                     | 0.65              |
| 23:DB:1979:U:O2'   | 23:DB:1980:G:H5'   | 1.96                     | 0.65              |
| 23:DB:2286:G:H1    | 48:D1:23:THR:CG2   | 2.10                     | 0.65              |
| 24:DV:25:LYS:HE2   | 24:DV:41:GLU:CB    | 2.27                     | 0.65              |
| 25:DC:224:MET:CA   | 25:DC:233:GLY:H    | 2.09                     | 0.65              |
| 31:DJ:41:LYS:HD2   | 31:DJ:44:TYR:HB3   | 1.79                     | 0.65              |
| 38:DQ:50:ARG:CZ    | 38:DQ:50:ARG:HA    | 2.26                     | 0.65              |
| 46:DZ:20:ASN:O     | 46:DZ:21:VAL:HB    | 1.94                     | 0.65              |
| 46:DZ:24:ILE:HD13  | 46:DZ:24:ILE:N     | 2.11                     | 0.65              |
| 1:AA:87:C:H2'      | 1:AA:88:U:H4'      | 1.76                     | 0.64              |
| 1:AA:190:A:H2'     | 1:AA:191:G:O4'     | 1.96                     | 0.64              |
| 1:AA:205:A:H2'     | 1:AA:206:C:H6      | 1.61                     | 0.64              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:946:A:H2'     | 1:AA:947:G:H8      | 1.60                     | 0.64              |
| 1:AA:997:U:O2'     | 1:AA:998:C:H5'     | 1.97                     | 0.64              |
| 2:AC:45:GLU:C      | 2:AC:46:LEU:HD12   | 2.22                     | 0.64              |
| 6:AG:44:SER:O      | 6:AG:48:THR:HG23   | 1.97                     | 0.64              |
| 12:AM:9:PRO:O      | 12:AM:44:ILE:HG12  | 1.97                     | 0.64              |
| 23:BB:144:A:H2'    | 23:BB:145:C:C6     | 2.29                     | 0.64              |
| 23:BB:1113:U:H5''  | 29:BG:1:SER:CA     | 2.27                     | 0.64              |
| 23:BB:1548:A:H2'   | 23:BB:1549:A:H8    | 1.63                     | 0.64              |
| 23:BB:2144:G:H22   | 23:BB:2148:G:H1'   | 1.62                     | 0.64              |
| 23:BB:2365:G:H4'   | 43:BW:65:LYS:NZ    | 2.12                     | 0.64              |
| 23:BB:2784:U:H2'   | 23:BB:2785:C:H6    | 1.61                     | 0.64              |
| 29:BG:70:LEU:HD12  | 29:BG:74:MET:HE3   | 1.78                     | 0.64              |
| 29:BG:84:LYS:HZ2   | 29:BG:85:LYS:N     | 1.95                     | 0.64              |
| 31:BJ:39:LYS:NZ    | 38:BQ:69:ARG:HD2   | 2.11                     | 0.64              |
| 32:BK:17:ARG:HD2   | 32:BK:18:ARG:H     | 1.62                     | 0.64              |
| 33:BL:111:ILE:HD13 | 33:BL:111:ILE:H    | 1.62                     | 0.64              |
| 46:BZ:66:ILE:HB    | 46:BZ:67:PRO:HD3   | 1.80                     | 0.64              |
| 1:CA:312:C:H2'     | 1:CA:313:A:H8      | 1.62                     | 0.64              |
| 1:CA:1072:G:H2'    | 1:CA:1073:U:C6     | 2.32                     | 0.64              |
| 5:CF:1:MET:SD      | 5:CF:67:PRO:HD3    | 2.37                     | 0.64              |
| 8:CI:98:ARG:HG2    | 8:CI:103:VAL:HG11  | 1.78                     | 0.64              |
| 20:CB:112:ARG:O    | 20:CB:116:LEU:HB2  | 1.97                     | 0.64              |
| 23:DB:93:G:H2'     | 23:DB:94:A:O4'     | 1.98                     | 0.64              |
| 23:DB:1099:G:O5'   | 52:DI:3:LYS:C      | 2.39                     | 0.64              |
| 23:DB:1820:U:H3    | 25:DC:197:ALA:CB   | 2.10                     | 0.64              |
| 23:DB:1821:A:H5'   | 25:DC:155:ARG:HH21 | 1.61                     | 0.64              |
| 23:DB:2051:A:H4'   | 26:DD:145:SER:HB2  | 1.80                     | 0.64              |
| 23:DB:2484:G:H1'   | 34:DM:119:LEU:HD12 | 1.80                     | 0.64              |
| 37:DP:50:ARG:HB2   | 37:DP:50:ARG:HH11  | 1.61                     | 0.64              |
| 46:DZ:17:SER:H     | 46:DZ:21:VAL:CG1   | 2.10                     | 0.64              |
| 1:AA:501:C:H2'     | 1:AA:502:A:C8      | 2.31                     | 0.64              |
| 1:AA:913:A:O2'     | 1:AA:914:A:O5'     | 2.13                     | 0.64              |
| 7:AH:64:TYR:HB3    | 7:AH:69:ALA:HA     | 1.79                     | 0.64              |
| 8:AI:18:VAL:HG22   | 8:AI:64:ILE:HG12   | 1.79                     | 0.64              |
| 18:AS:4:LEU:HD13   | 18:AS:9:PHE:N      | 2.10                     | 0.64              |
| 20:AB:119:GLN:O    | 20:AB:124:THR:HG23 | 1.97                     | 0.64              |
| 23:BB:396:G:H4'    | 46:BZ:28:VAL:CG2   | 2.25                     | 0.64              |
| 23:BB:1447:C:H2'   | 23:BB:1448:G:H8    | 1.61                     | 0.64              |
| 23:BB:1935:G:H1'   | 23:BB:1964:G:N2    | 2.12                     | 0.64              |
| 23:BB:2814:A:H2'   | 23:BB:2815:C:C6    | 2.32                     | 0.64              |
| 26:BD:38:LYS:HE2   | 26:BD:38:LYS:H     | 1.62                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:BD:115:GLY:CA  | 26:BD:165:MET:HG3  | 2.27                     | 0.64              |
| 27:BE:141:MET:SD  | 27:BE:143:LEU:HB2  | 2.37                     | 0.64              |
| 28:BF:102:LEU:C   | 28:BF:107:VAL:HG23 | 2.23                     | 0.64              |
| 30:BH:6:LEU:HD12  | 30:BH:15:LEU:HA    | 1.78                     | 0.64              |
| 35:BN:99:LYS:HE2  | 47:B0:38:LEU:O     | 1.96                     | 0.64              |
| 46:BZ:36:VAL:HA   | 46:BZ:42:PRO:CB    | 2.23                     | 0.64              |
| 50:B3:29:ARG:HA   | 50:B3:33:THR:HG23  | 1.79                     | 0.64              |
| 52:BI:109:ALA:HB1 | 52:BI:124:MET:HG3  | 1.79                     | 0.64              |
| 1:CA:190:A:H2'    | 1:CA:191:G:O4'     | 1.96                     | 0.64              |
| 5:CF:66:ALA:HB1   | 5:CF:67:PRO:HD2    | 1.79                     | 0.64              |
| 23:DB:536:G:C5'   | 38:DQ:52:ARG:HH22  | 2.10                     | 0.64              |
| 23:DB:1149:G:H2'  | 23:DB:1150:C:H6    | 1.61                     | 0.64              |
| 23:DB:1179:G:H2'  | 23:DB:1180:U:C6    | 2.32                     | 0.64              |
| 23:DB:2025:C:H2'  | 23:DB:2026:U:C6    | 2.33                     | 0.64              |
| 23:DB:2852:G:H2'  | 23:DB:2853:C:C6    | 2.32                     | 0.64              |
| 29:DG:10:VAL:N    | 29:DG:11:PRO:HD3   | 2.12                     | 0.64              |
| 34:DM:41:LEU:O    | 34:DM:93:VAL:HB    | 1.97                     | 0.64              |
| 1:AA:372:C:H1'    | 1:AA:373:A:OP2     | 1.97                     | 0.64              |
| 1:AA:376:G:H5''   | 15:AP:5:ARG:CB     | 2.26                     | 0.64              |
| 1:AA:389:A:H3'    | 1:AA:390:U:H6      | 1.62                     | 0.64              |
| 15:AP:4:ILE:HD12  | 15:AP:66:THR:O     | 1.97                     | 0.64              |
| 23:BB:6:A:H2'     | 23:BB:7:G:C8       | 2.33                     | 0.64              |
| 23:BB:142:A:N3    | 41:BT:2:ILE:HG23   | 2.11                     | 0.64              |
| 23:BB:1515:A:H2'  | 23:BB:1516:G:O4'   | 1.97                     | 0.64              |
| 23:BB:2287:A:O2'  | 23:BB:2288:A:H2'   | 1.98                     | 0.64              |
| 25:BC:65:ASP:OD2  | 25:BC:101:ARG:HB3  | 1.98                     | 0.64              |
| 26:BD:37:VAL:HG22 | 26:BD:46:ARG:NE    | 2.11                     | 0.64              |
| 31:BJ:39:LYS:HE2  | 31:BJ:39:LYS:HA    | 1.79                     | 0.64              |
| 34:BM:96:ILE:HG23 | 34:BM:97:GLN:N     | 2.10                     | 0.64              |
| 43:BW:48:ALA:HA   | 43:BW:54:ARG:N     | 2.10                     | 0.64              |
| 46:BZ:32:LEU:HD22 | 46:BZ:33:ASN:N     | 2.12                     | 0.64              |
| 50:B3:26:ALA:HB1  | 50:B3:29:ARG:CG    | 2.26                     | 0.64              |
| 1:CA:89:U:H2'     | 1:CA:90:C:C6       | 2.33                     | 0.64              |
| 1:CA:952:U:H2'    | 1:CA:953:G:H8      | 1.62                     | 0.64              |
| 1:CA:1080:A:H4'   | 4:CE:20:VAL:HG21   | 1.78                     | 0.64              |
| 1:CA:1244:G:H2'   | 1:CA:1245:C:C6     | 2.32                     | 0.64              |
| 1:CA:1373:G:H5''  | 6:CG:35:LYS:HB2    | 1.78                     | 0.64              |
| 2:CC:2:GLN:N      | 2:CC:2:GLN:HE21    | 1.96                     | 0.64              |
| 5:CF:29:ILE:HG22  | 5:CF:34:GLY:HA3    | 1.78                     | 0.64              |
| 12:CM:102:LYS:HB2 | 12:CM:102:LYS:NZ   | 2.12                     | 0.64              |
| 23:DB:418:C:H2'   | 23:DB:419:U:C6     | 2.33                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DB:1354:A:H2'   | 23:DB:1355:G:O4'  | 1.97                     | 0.64              |
| 23:DB:2197:U:O2'   | 23:DB:2198:A:H2'  | 1.97                     | 0.64              |
| 36:DO:30:ARG:HG2   | 36:DO:31:THR:H    | 1.62                     | 0.64              |
| 1:AA:441:A:H61     | 1:AA:493:A:H62    | 1.45                     | 0.64              |
| 1:AA:1294:G:H2'    | 1:AA:1295:U:H6    | 1.60                     | 0.64              |
| 1:AA:1513:A:H2'    | 1:AA:1514:G:C8    | 2.32                     | 0.64              |
| 22:BA:20:G:H2'     | 22:BA:21:G:C8     | 2.32                     | 0.64              |
| 23:BB:840:C:O2'    | 23:BB:841:G:H5'   | 1.97                     | 0.64              |
| 23:BB:1181:U:H2'   | 23:BB:1182:G:H8   | 1.62                     | 0.64              |
| 23:BB:1387:A:H2'   | 23:BB:1388:G:H8   | 1.63                     | 0.64              |
| 23:BB:2155:U:H2'   | 23:BB:2156:G:O4'  | 1.98                     | 0.64              |
| 25:BC:67:LYS:HG3   | 25:BC:68:ARG:N    | 2.12                     | 0.64              |
| 27:BE:145:ASP:C    | 27:BE:147:LEU:H   | 2.04                     | 0.64              |
| 30:BH:5:LEU:HD13   | 30:BH:37:VAL:HG11 | 1.80                     | 0.64              |
| 32:BK:5:GLN:O      | 32:BK:21:CYS:HB3  | 1.98                     | 0.64              |
| 35:BN:118:ARG:HG2  | 47:B0:52:LYS:HE2  | 1.79                     | 0.64              |
| 39:BR:47:VAL:HG22  | 39:BR:48:LYS:HG2  | 1.79                     | 0.64              |
| 44:BX:19:LEU:HA    | 44:BX:22:LEU:HB2  | 1.78                     | 0.64              |
| 47:B0:52:LYS:HA    | 47:B0:52:LYS:NZ   | 2.12                     | 0.64              |
| 52:BI:20:SER:O     | 52:BI:25:PRO:HD2  | 1.98                     | 0.64              |
| 1:CA:1001:C:H2'    | 1:CA:1002:G:C8    | 2.33                     | 0.64              |
| 2:CC:2:GLN:HE21    | 2:CC:2:GLN:H      | 1.44                     | 0.64              |
| 18:CS:41:PRO:HA    | 18:CS:44:ILE:HG13 | 1.79                     | 0.64              |
| 20:CB:15:PHE:HB3   | 20:CB:42:LEU:HD11 | 1.78                     | 0.64              |
| 23:DB:2814:A:H2'   | 23:DB:2815:C:C6   | 2.32                     | 0.64              |
| 32:DK:61:VAL:HG13  | 32:DK:87:LEU:HD11 | 1.80                     | 0.64              |
| 48:D1:24:LYS:HB2   | 48:D1:24:LYS:HZ2  | 1.62                     | 0.64              |
| 1:AA:518:C:H2'     | 1:AA:530:G:C8     | 2.31                     | 0.64              |
| 7:AH:36:ALA:HA     | 7:AH:39:LEU:HD12  | 1.79                     | 0.64              |
| 10:AK:95:THR:HG23  | 10:AK:96:ILE:H    | 1.62                     | 0.64              |
| 23:BB:28:A:H61     | 23:BB:512:G:H1'   | 1.62                     | 0.64              |
| 23:BB:639:U:H2'    | 23:BB:640:C:C6    | 2.33                     | 0.64              |
| 23:BB:855:G:H21    | 43:BW:23:LYS:CD   | 2.09                     | 0.64              |
| 23:BB:2575:C:H5''  | 26:BD:149:ASN:H   | 1.61                     | 0.64              |
| 23:BB:2880:C:H1'   | 35:BN:92:GLY:O    | 1.98                     | 0.64              |
| 25:BC:227:VAL:HG12 | 25:BC:228:ASP:OD1 | 1.98                     | 0.64              |
| 26:BD:120:GLY:N    | 26:BD:123:LYS:HG3 | 2.13                     | 0.64              |
| 28:BF:12:VAL:HG13  | 28:BF:27:VAL:HG21 | 1.79                     | 0.64              |
| 28:BF:18:GLU:O     | 28:BF:19:PHE:HB3  | 1.97                     | 0.64              |
| 35:BN:7:GLY:O      | 35:BN:8:ARG:HB2   | 1.96                     | 0.64              |
| 48:B1:34:GLU:OE1   | 48:B1:36:LYS:HE2  | 1.97                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:83:C:H4'      | 1:CA:83:C:OP1      | 1.98                     | 0.64              |
| 1:CA:1103:C:O2     | 20:CB:105:THR:HG21 | 1.97                     | 0.64              |
| 23:DB:86:G:OP1     | 42:DU:30:SER:HB3   | 1.97                     | 0.64              |
| 23:DB:1690:A:H2'   | 23:DB:1691:C:O4'   | 1.98                     | 0.64              |
| 23:DB:1935:G:H1'   | 23:DB:1964:G:N2    | 2.12                     | 0.64              |
| 25:DC:29:PHE:O     | 25:DC:29:PHE:CD1   | 2.50                     | 0.64              |
| 25:DC:107:LYS:HE3  | 25:DC:108:GLY:N    | 2.05                     | 0.64              |
| 27:DE:115:GLN:HB3  | 27:DE:117:ARG:NH1  | 2.12                     | 0.64              |
| 28:DF:56:LEU:HD22  | 28:DF:88:VAL:HG21  | 1.80                     | 0.64              |
| 30:DH:127:GLU:HA   | 30:DH:144:VAL:O    | 1.97                     | 0.64              |
| 34:DM:131:VAL:HG22 | 34:DM:133:LYS:N    | 2.12                     | 0.64              |
| 39:DR:63:VAL:HG22  | 39:DR:64:VAL:N     | 2.07                     | 0.64              |
| 51:D4:23:ILE:CD1   | 51:D4:24:ARG:H     | 2.11                     | 0.64              |
| 8:AI:49:GLN:NE2    | 8:AI:79:ARG:HD2    | 2.13                     | 0.64              |
| 12:AM:13:HIS:HB2   | 12:AM:16:ILE:HG22  | 1.79                     | 0.64              |
| 12:AM:68:LEU:O     | 12:AM:72:ILE:HD13  | 1.97                     | 0.64              |
| 18:AS:50:VAL:O     | 18:AS:56:HIS:HA    | 1.97                     | 0.64              |
| 23:BB:13:A:H61     | 23:BB:525:U:H2'    | 1.63                     | 0.64              |
| 23:BB:196:A:H2'    | 23:BB:196:A:N3     | 2.12                     | 0.64              |
| 23:BB:923:G:H1'    | 43:BW:23:LYS:CD    | 2.23                     | 0.64              |
| 23:BB:1225:G:H5''  | 39:BR:78:ARG:HH22  | 1.61                     | 0.64              |
| 25:BC:171:VAL:HB   | 25:BC:182:LYS:HB3  | 1.80                     | 0.64              |
| 27:BE:58:LYS:O     | 27:BE:58:LYS:HD3   | 1.97                     | 0.64              |
| 28:BF:75:GLY:O     | 28:BF:76:PHE:HB2   | 1.97                     | 0.64              |
| 30:BH:83:LYS:HB3   | 30:BH:91:PHE:CD1   | 2.31                     | 0.64              |
| 33:BL:109:LYS:HA   | 33:BL:126:ARG:CA   | 2.27                     | 0.64              |
| 39:BR:90:ARG:HH11  | 39:BR:91:GLN:H     | 1.46                     | 0.64              |
| 41:BT:3:ARG:HH22   | 44:BX:19:LEU:HD22  | 1.61                     | 0.64              |
| 47:B0:28:SER:HB2   | 47:B0:34:GLY:N     | 2.12                     | 0.64              |
| 4:CE:137:ARG:HH11  | 4:CE:137:ARG:HG2   | 1.63                     | 0.64              |
| 11:CL:43:LYS:CB    | 11:CL:44:PRO:HD2   | 2.17                     | 0.64              |
| 12:CM:14:ALA:HB3   | 12:CM:40:GLU:HA    | 1.78                     | 0.64              |
| 15:CP:28:ARG:CD    | 15:CP:29:ASN:H     | 2.09                     | 0.64              |
| 23:DB:64:A:H2'     | 23:DB:65:U:C6      | 2.32                     | 0.64              |
| 23:DB:321:U:OP2    | 27:DE:130:LYS:HG3  | 1.98                     | 0.64              |
| 23:DB:2196:C:O2'   | 23:DB:2197:U:H5'   | 1.97                     | 0.64              |
| 23:DB:2238:G:H2'   | 23:DB:2238:G:N3    | 2.13                     | 0.64              |
| 23:DB:2365:G:H4'   | 43:DW:65:LYS:HD2   | 1.80                     | 0.64              |
| 33:DL:39:LYS:HA    | 33:DL:39:LYS:NZ    | 2.13                     | 0.64              |
| 38:DQ:47:ARG:HH12  | 38:DQ:50:ARG:HG3   | 1.62                     | 0.64              |
| 2:AC:39:ARG:HG3    | 2:AC:54:ILE:HG21   | 1.79                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:AG:3:ARG:HB3     | 6:AG:3:ARG:HH11    | 1.63                     | 0.64              |
| 6:AG:4:ARG:HE      | 6:AG:5:VAL:N       | 1.94                     | 0.64              |
| 10:AK:19:VAL:HG12  | 10:AK:82:GLU:HB2   | 1.80                     | 0.64              |
| 10:AK:52:ARG:HD2   | 10:AK:53:GLY:N     | 2.13                     | 0.64              |
| 16:AQ:10:ARG:HA    | 16:AQ:10:ARG:HE    | 1.63                     | 0.64              |
| 23:BB:796:C:H2'    | 23:BB:797:G:H8     | 1.62                     | 0.64              |
| 23:BB:1198:U:H2'   | 23:BB:1199:U:C6    | 2.32                     | 0.64              |
| 23:BB:1459:G:O2'   | 23:BB:1460:U:H5'   | 1.98                     | 0.64              |
| 23:BB:1813:G:N2    | 25:BC:51:ARG:HG2   | 2.12                     | 0.64              |
| 23:BB:2104:C:H2'   | 23:BB:2105:U:C5    | 2.32                     | 0.64              |
| 23:BB:2443:C:H2'   | 23:BB:2444:G:C8    | 2.31                     | 0.64              |
| 25:BC:16:VAL:HA    | 25:BC:17:LYS:HZ3   | 1.63                     | 0.64              |
| 25:BC:250:GLN:HB3  | 25:BC:252:LYS:HE2  | 1.78                     | 0.64              |
| 26:BD:2:ILE:HG13   | 26:BD:3:GLY:H      | 1.62                     | 0.64              |
| 26:BD:62:LYS:H     | 26:BD:62:LYS:HD3   | 1.62                     | 0.64              |
| 29:BG:116:LEU:HD21 | 29:BG:120:ILE:HB   | 1.79                     | 0.64              |
| 46:BZ:36:VAL:HG22  | 46:BZ:42:PRO:HG3   | 1.78                     | 0.64              |
| 52:BI:85:ILE:HD13  | 52:BI:137:LEU:HD21 | 1.78                     | 0.64              |
| 1:CA:1402:C:H2'    | 1:CA:1403:C:O4'    | 1.98                     | 0.64              |
| 2:CC:149:LYS:HB2   | 2:CC:168:ARG:HG3   | 1.80                     | 0.64              |
| 3:CD:28:ASP:CB     | 3:CD:33:ILE:HD12   | 2.28                     | 0.64              |
| 10:CK:61:ALA:O     | 10:CK:64:VAL:HG22  | 1.97                     | 0.64              |
| 12:CM:47:LEU:HD23  | 12:CM:47:LEU:H     | 1.63                     | 0.64              |
| 12:CM:102:LYS:HZ2  | 12:CM:103:THR:HG23 | 1.63                     | 0.64              |
| 22:DA:51:G:H2'     | 22:DA:52:A:H5''    | 1.78                     | 0.64              |
| 23:DB:639:U:H2'    | 23:DB:640:C:C6     | 2.33                     | 0.64              |
| 23:DB:796:C:H2'    | 23:DB:797:G:H8     | 1.62                     | 0.64              |
| 23:DB:813:U:H2'    | 23:DB:814:C:H6     | 1.63                     | 0.64              |
| 26:DD:3:GLY:C      | 26:DD:4:LEU:HD13   | 2.23                     | 0.64              |
| 26:DD:128:ARG:HD3  | 26:DD:128:ARG:N    | 2.13                     | 0.64              |
| 31:DJ:64:VAL:HG12  | 31:DJ:65:THR:N     | 2.11                     | 0.64              |
| 31:DJ:98:GLU:O     | 31:DJ:102:GLU:HG2  | 1.98                     | 0.64              |
| 37:DP:59:THR:HG23  | 37:DP:76:HIS:CD2   | 2.31                     | 0.64              |
| 39:DR:80:ARG:O     | 39:DR:80:ARG:HG3   | 1.97                     | 0.64              |
| 43:DW:13:ARG:H     | 43:DW:13:ARG:NE    | 1.90                     | 0.64              |
| 49:D2:34:ARG:HD2   | 49:D2:43:THR:OG1   | 1.97                     | 0.64              |
| 1:AA:411:A:O2'     | 1:AA:412:A:H4'     | 1.98                     | 0.64              |
| 1:AA:1077:G:N2     | 1:AA:1079:G:H3'    | 2.13                     | 0.64              |
| 8:AI:20:ILE:HG23   | 8:AI:60:LEU:HD13   | 1.79                     | 0.64              |
| 20:AB:198:VAL:HG22 | 20:AB:200:PRO:HD3  | 1.79                     | 0.64              |
| 23:BB:674:G:H5''   | 27:BE:71:GLY:N     | 2.13                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:1181:U:H2'   | 23:BB:1182:G:C8    | 2.32                     | 0.64              |
| 23:BB:1354:A:H2'   | 23:BB:1355:G:O4'   | 1.97                     | 0.64              |
| 23:BB:1360:G:H2'   | 23:BB:1361:G:H5'   | 1.79                     | 0.64              |
| 23:BB:2743:U:H3'   | 23:BB:2744:G:H5''  | 1.80                     | 0.64              |
| 28:BF:151:LEU:HD23 | 28:BF:153:ILE:HD11 | 1.80                     | 0.64              |
| 31:BJ:35:ARG:HA    | 31:BJ:35:ARG:NE    | 2.13                     | 0.64              |
| 33:BL:64:PHE:N     | 50:B3:24:LYS:HZ2   | 1.96                     | 0.64              |
| 41:BT:88:LYS:CG    | 41:BT:89:GLU:H     | 2.06                     | 0.64              |
| 46:BZ:5:ILE:HB     | 46:BZ:51:VAL:HG13  | 1.79                     | 0.64              |
| 1:CA:376:G:H5''    | 15:CP:5:ARG:HD3    | 1.79                     | 0.64              |
| 5:CF:43:GLY:HA2    | 5:CF:58:HIS:CD2    | 2.33                     | 0.64              |
| 12:CM:89:ARG:NH1   | 12:CM:101:THR:HG21 | 2.12                     | 0.64              |
| 15:CP:57:ILE:C     | 15:CP:57:ILE:HD13  | 2.22                     | 0.64              |
| 22:DA:7:G:H5''     | 36:DO:29:HIS:NE2   | 2.13                     | 0.64              |
| 23:DB:828:U:H4'    | 23:DB:831:G:N1     | 2.13                     | 0.64              |
| 23:DB:1007:C:H5''  | 31:DJ:37:ARG:NH1   | 2.13                     | 0.64              |
| 23:DB:1814:G:C4'   | 25:DC:51:ARG:HG2   | 2.28                     | 0.64              |
| 23:DB:2334:U:N3    | 43:DW:74:LYS:HE2   | 2.10                     | 0.64              |
| 25:DC:20:ASN:HB2   | 25:DC:202:ARG:HH11 | 1.63                     | 0.64              |
| 25:DC:52:HIS:O     | 25:DC:53:ILE:HB    | 1.96                     | 0.64              |
| 26:DD:197:THR:HG23 | 26:DD:198:GLY:N    | 2.07                     | 0.64              |
| 27:DE:108:ILE:HG22 | 27:DE:180:LEU:HD13 | 1.79                     | 0.64              |
| 29:DG:148:ARG:HA   | 29:DG:161:VAL:CG1  | 2.28                     | 0.64              |
| 32:DK:35:VAL:HA    | 32:DK:62:VAL:O     | 1.98                     | 0.64              |
| 46:DZ:48:GLN:HB3   | 46:DZ:51:VAL:CG2   | 2.28                     | 0.64              |
| 1:AA:190:A:H8      | 1:AA:190:A:O5'     | 1.80                     | 0.64              |
| 1:AA:674:G:H2'     | 1:AA:675:A:H8      | 1.63                     | 0.64              |
| 1:AA:1111:A:O2'    | 1:AA:1112:C:H6     | 1.81                     | 0.64              |
| 1:AA:1278:G:H4'    | 1:AA:1279:G:O5'    | 1.98                     | 0.64              |
| 6:AG:23:ALA:O      | 6:AG:26:VAL:HG22   | 1.98                     | 0.64              |
| 9:AJ:7:ARG:HA      | 9:AJ:75:ASP:HB2    | 1.78                     | 0.64              |
| 9:AJ:65:TYR:HB3    | 13:AN:95:LEU:HD11  | 1.80                     | 0.64              |
| 16:AQ:59:GLU:H     | 16:AQ:74:LEU:CD2   | 2.11                     | 0.64              |
| 23:BB:1117:C:H2'   | 23:BB:1118:C:C6    | 2.32                     | 0.64              |
| 23:BB:1690:A:H2'   | 23:BB:1691:C:O4'   | 1.98                     | 0.64              |
| 23:BB:1812:U:H1'   | 25:BC:45:ASN:OD1   | 1.98                     | 0.64              |
| 30:BH:112:LYS:O    | 30:BH:112:LYS:HD2  | 1.98                     | 0.64              |
| 34:BM:109:PRO:HA   | 34:BM:112:LEU:HD22 | 1.80                     | 0.64              |
| 35:BN:113:ILE:O    | 35:BN:114:GLU:HB2  | 1.96                     | 0.64              |
| 36:BO:109:ALA:HA   | 36:BO:112:GLU:OE1  | 1.98                     | 0.64              |
| 42:BU:11:ILE:HB    | 42:BU:69:VAL:HB    | 1.78                     | 0.64              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 42:BU:43:LYS:HD2  | 42:BU:44:HIS:N     | 2.13                     | 0.64              |
| 45:BY:4:ILE:HG12  | 45:BY:5:LYS:HG3    | 1.80                     | 0.64              |
| 1:CA:1097:C:H2'   | 1:CA:1098:C:H6     | 1.61                     | 0.64              |
| 1:CA:1306:A:O2'   | 12:CM:107:THR:HG21 | 1.98                     | 0.64              |
| 7:CH:102:VAL:HG23 | 7:CH:125:ILE:HB    | 1.80                     | 0.64              |
| 12:CM:78:ARG:HG3  | 28:DF:111:ARG:HH11 | 1.62                     | 0.64              |
| 15:CP:40:ASN:HD21 | 15:CP:42:ILE:HG12  | 1.63                     | 0.64              |
| 19:CT:52:GLU:O    | 19:CT:56:ILE:HD13  | 1.98                     | 0.64              |
| 23:DB:1319:C:O2'  | 23:DB:1320:C:H5'   | 1.98                     | 0.64              |
| 23:DB:1387:A:H2'  | 23:DB:1388:G:H8    | 1.63                     | 0.64              |
| 23:DB:2811:G:H5'  | 26:DD:62:LYS:NZ    | 2.13                     | 0.64              |
| 23:DB:2820:A:C4'  | 35:DN:4:ARG:HG3    | 2.27                     | 0.64              |
| 24:DV:9:ARG:HH22  | 24:DV:16:ALA:HB1   | 1.61                     | 0.64              |
| 26:DD:140:HIS:O   | 26:DD:141:ARG:HG2  | 1.97                     | 0.64              |
| 27:DE:31:VAL:HG21 | 27:DE:104:ALA:HB2  | 1.79                     | 0.64              |
| 33:DL:59:ARG:HA   | 50:D3:11:LYS:HZ1   | 1.62                     | 0.64              |
| 35:DN:8:ARG:NH1   | 35:DN:46:ARG:HG3   | 2.13                     | 0.64              |
| 1:AA:1488:G:O2'   | 1:AA:1489:G:H5'    | 1.98                     | 0.64              |
| 3:AD:88:ASN:O     | 3:AD:92:LEU:HD23   | 1.97                     | 0.64              |
| 7:AH:8:ASP:O      | 7:AH:12:ARG:HG3    | 1.98                     | 0.64              |
| 9:AJ:25:ILE:HG23  | 9:AJ:29:ALA:HB3    | 1.79                     | 0.64              |
| 20:AB:37:VAL:HG22 | 20:AB:38:HIS:N     | 2.13                     | 0.64              |
| 20:AB:148:GLY:O   | 20:AB:151:LYS:HE2  | 1.98                     | 0.64              |
| 23:BB:1188:U:H4'  | 39:BR:83:TYR:CB    | 2.27                     | 0.64              |
| 23:BB:1973:G:H2'  | 23:BB:1974:C:C6    | 2.33                     | 0.64              |
| 27:BE:1:MET:O     | 27:BE:14:VAL:HG22  | 1.98                     | 0.64              |
| 33:BL:132:ARG:O   | 33:BL:136:GLU:HB3  | 1.98                     | 0.64              |
| 48:B1:13:SER:H    | 48:B1:50:GLU:HA    | 1.62                     | 0.64              |
| 51:B4:14:CYS:SG   | 51:B4:25:VAL:HG12  | 2.38                     | 0.64              |
| 1:CA:89:U:H2'     | 1:CA:90:C:H6       | 1.62                     | 0.64              |
| 1:CA:451:A:H5'    | 15:CP:70:ARG:NH2   | 2.12                     | 0.64              |
| 1:CA:677:U:H3     | 1:CA:713:G:H22     | 1.47                     | 0.64              |
| 1:CA:1237:C:H3'   | 1:CA:1238:A:H5'    | 1.78                     | 0.64              |
| 1:CA:1526:G:P     | 21:CU:38:GLU:HB2   | 2.38                     | 0.64              |
| 18:CS:27:LYS:HZ3  | 18:CS:27:LYS:HB3   | 1.63                     | 0.64              |
| 23:DB:7:G:H2'     | 23:DB:8:C:C6       | 2.33                     | 0.64              |
| 23:DB:37:C:O2'    | 23:DB:38:A:H5'     | 1.98                     | 0.64              |
| 23:DB:118:A:OP2   | 23:DB:119:A:H2'    | 1.98                     | 0.64              |
| 23:DB:784:G:H5''  | 25:DC:225:ASN:HD21 | 1.63                     | 0.64              |
| 23:DB:1447:C:H2'  | 23:DB:1448:G:H8    | 1.61                     | 0.64              |
| 23:DB:2249:U:H4'  | 23:DB:2275:C:C5    | 2.33                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DC:179:GLU:HG3  | 25:DC:266:ILE:HG22 | 1.80                     | 0.64              |
| 26:DD:25:THR:HA    | 26:DD:188:LEU:HD12 | 1.79                     | 0.64              |
| 30:DH:108:VAL:HG12 | 30:DH:110:VAL:HB   | 1.80                     | 0.64              |
| 33:DL:78:ARG:HB3   | 33:DL:78:ARG:NH1   | 2.13                     | 0.64              |
| 38:DQ:91:ARG:HA    | 38:DQ:94:LEU:HD21  | 1.79                     | 0.64              |
| 43:DW:67:LYS:HD3   | 43:DW:68:PHE:H     | 1.62                     | 0.64              |
| 50:D3:54:LEU:HA    | 50:D3:57:VAL:HG12  | 1.80                     | 0.64              |
| 1:AA:203:G:H1'     | 1:AA:465:A:N6      | 2.13                     | 0.63              |
| 1:AA:1412:C:H2'    | 1:AA:1413:A:H8     | 1.61                     | 0.63              |
| 3:AD:186:GLU:O     | 3:AD:190:LEU:HD13  | 1.98                     | 0.63              |
| 8:AI:30:ASN:ND2    | 8:AI:65:THR:HA     | 2.13                     | 0.63              |
| 13:AN:15:LEU:HD12  | 13:AN:16:ALA:N     | 2.13                     | 0.63              |
| 23:BB:704:G:H1'    | 23:BB:727:A:N6     | 2.12                     | 0.63              |
| 23:BB:1219:U:H2'   | 23:BB:1220:G:H8    | 1.63                     | 0.63              |
| 23:BB:1821:A:H5'   | 25:BC:155:ARG:HH21 | 1.62                     | 0.63              |
| 29:BG:23:ILE:O     | 29:BG:33:THR:HA    | 1.97                     | 0.63              |
| 31:BJ:73:VAL:HG23  | 31:BJ:74:TYR:H     | 1.63                     | 0.63              |
| 32:BK:108:ARG:HA   | 32:BK:116:ILE:HG21 | 1.80                     | 0.63              |
| 34:BM:86:LYS:N     | 34:BM:86:LYS:HD2   | 2.13                     | 0.63              |
| 35:BN:28:LEU:HD22  | 35:BN:48:VAL:HG21  | 1.80                     | 0.63              |
| 37:BP:47:ILE:HA    | 37:BP:63:ILE:HG23  | 1.79                     | 0.63              |
| 40:BS:27:LYS:HD2   | 40:BS:27:LYS:N     | 2.09                     | 0.63              |
| 46:BZ:49:ARG:C     | 46:BZ:51:VAL:H     | 2.07                     | 0.63              |
| 1:CA:203:G:H1'     | 1:CA:465:A:N6      | 2.13                     | 0.63              |
| 1:CA:674:G:H2'     | 1:CA:675:A:H8      | 1.63                     | 0.63              |
| 10:CK:121:ARG:HE   | 21:CU:34:ARG:HG2   | 1.62                     | 0.63              |
| 23:DB:878:A:N3     | 23:DB:878:A:H2'    | 2.12                     | 0.63              |
| 23:DB:2080:A:H2'   | 23:DB:2081:U:C6    | 2.33                     | 0.63              |
| 23:DB:2784:U:H2'   | 23:DB:2785:C:C6    | 2.33                     | 0.63              |
| 26:DD:146:ILE:HD12 | 26:DD:146:ILE:H    | 1.64                     | 0.63              |
| 34:DM:57:VAL:HG12  | 34:DM:58:LYS:N     | 2.09                     | 0.63              |
| 34:DM:127:LYS:HZ3  | 34:DM:129:THR:H    | 1.46                     | 0.63              |
| 43:DW:43:LYS:HD2   | 43:DW:76:ARG:HA    | 1.79                     | 0.63              |
| 51:D4:10:LEU:HB2   | 51:D4:25:VAL:HG23  | 1.80                     | 0.63              |
| 52:DI:2:LYS:C      | 52:DI:3:LYS:HD2    | 2.23                     | 0.63              |
| 8:AI:122:ARG:HG3   | 8:AI:122:ARG:HH11  | 1.64                     | 0.63              |
| 22:BA:76:G:H2'     | 22:BA:77:U:H6      | 1.63                     | 0.63              |
| 23:BB:125:A:H3'    | 23:BB:126:A:H5'    | 1.79                     | 0.63              |
| 23:BB:298:G:H2'    | 23:BB:339:U:O4     | 1.98                     | 0.63              |
| 23:BB:1192:G:O2'   | 23:BB:1193:G:H5'   | 1.98                     | 0.63              |
| 23:BB:1205:A:H4'   | 23:BB:1206:G:OP2   | 1.96                     | 0.63              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BC:141:HIS:CB   | 25:BC:190:THR:HB   | 2.29                     | 0.63              |
| 26:BD:23:PRO:HB3   | 26:BD:189:VAL:H    | 1.63                     | 0.63              |
| 48:B1:9:LYS:N      | 48:B1:9:LYS:HD2    | 2.14                     | 0.63              |
| 50:B3:41:ARG:HD3   | 50:B3:43:LEU:H     | 1.63                     | 0.63              |
| 1:CA:93:U:H2'      | 1:CA:94:G:H5'      | 1.79                     | 0.63              |
| 1:CA:1084:G:H5'    | 1:CA:1102:A:OP2    | 1.98                     | 0.63              |
| 1:CA:1404:C:H2'    | 1:CA:1405:G:C8     | 2.33                     | 0.63              |
| 23:DB:418:C:H2'    | 23:DB:419:U:H6     | 1.63                     | 0.63              |
| 23:DB:651:G:OP1    | 50:D3:18:LYS:HG2   | 1.97                     | 0.63              |
| 23:DB:2108:A:H2'   | 23:DB:2108:A:N3    | 2.13                     | 0.63              |
| 32:DK:107:LEU:HD21 | 32:DK:115:ILE:HD13 | 1.79                     | 0.63              |
| 35:DN:30:ARG:NH1   | 35:DN:74:GLU:HG2   | 2.14                     | 0.63              |
| 36:DO:17:LYS:HD2   | 36:DO:92:PHE:CD2   | 2.33                     | 0.63              |
| 40:DS:29:VAL:O     | 40:DS:33:LEU:HD23  | 1.98                     | 0.63              |
| 41:DT:24:MET:HE3   | 41:DT:24:MET:N     | 2.13                     | 0.63              |
| 52:DI:17:ALA:C     | 52:DI:19:PRO:HD3   | 2.23                     | 0.63              |
| 1:AA:524:G:H2'     | 1:AA:525:C:C6      | 2.34                     | 0.63              |
| 1:AA:677:U:H3      | 1:AA:713:G:H22     | 1.46                     | 0.63              |
| 7:AH:11:THR:HA     | 7:AH:14:ARG:NH1    | 2.12                     | 0.63              |
| 21:AU:7:GLU:OE2    | 21:AU:15:LEU:HD22  | 1.98                     | 0.63              |
| 23:BB:1060:U:H5    | 52:BI:131:THR:HG22 | 1.63                     | 0.63              |
| 23:BB:2025:C:H2'   | 23:BB:2026:U:C6    | 2.33                     | 0.63              |
| 23:BB:2070:A:H2'   | 23:BB:2071:A:C8    | 2.33                     | 0.63              |
| 25:BC:140:VAL:HG23 | 25:BC:141:HIS:H    | 1.64                     | 0.63              |
| 27:BE:132:LYS:HB2  | 27:BE:132:LYS:NZ   | 2.13                     | 0.63              |
| 30:BH:11:ASN:HD22  | 30:BH:12:LEU:H     | 1.46                     | 0.63              |
| 30:BH:83:LYS:HB2   | 30:BH:92:GLY:H     | 1.63                     | 0.63              |
| 35:BN:70:THR:HG21  | 35:BN:75:ILE:HG22  | 1.80                     | 0.63              |
| 35:BN:75:ILE:HD13  | 35:BN:75:ILE:O     | 1.99                     | 0.63              |
| 42:BU:35:VAL:HG12  | 42:BU:36:GLU:N     | 2.12                     | 0.63              |
| 46:BZ:59:ARG:HE    | 46:BZ:62:LYS:HD2   | 1.63                     | 0.63              |
| 46:BZ:70:LYS:N     | 46:BZ:70:LYS:HE2   | 2.12                     | 0.63              |
| 1:CA:411:A:O2'     | 1:CA:412:A:H4'     | 1.98                     | 0.63              |
| 1:CA:441:A:H61     | 1:CA:493:A:H62     | 1.45                     | 0.63              |
| 1:CA:985:C:H2'     | 1:CA:986:U:C6      | 2.33                     | 0.63              |
| 8:CI:86:LEU:HB3    | 8:CI:93:LEU:HD13   | 1.80                     | 0.63              |
| 8:CI:113:LYS:HA    | 8:CI:120:ALA:HB2   | 1.79                     | 0.63              |
| 11:CL:85:ARG:NH1   | 11:CL:93:ARG:HB3   | 2.13                     | 0.63              |
| 23:DB:588:U:H5'    | 33:DL:29:LYS:HZ2   | 1.62                     | 0.63              |
| 23:DB:907:G:H5'    | 34:DM:24:THR:HG21  | 1.80                     | 0.63              |
| 23:DB:1442:U:H2'   | 23:DB:1443:U:C6    | 2.33                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DB:1485:U:H2'   | 23:DB:1486:U:H6   | 1.63                     | 0.63              |
| 23:DB:2361:G:H5''  | 50:D3:27:ASN:HB2  | 1.79                     | 0.63              |
| 25:DC:75:ALA:HB2   | 25:DC:95:TYR:CD1  | 2.33                     | 0.63              |
| 25:DC:237:ARG:C    | 25:DC:237:ARG:HE  | 2.07                     | 0.63              |
| 27:DE:42:GLY:O     | 27:DE:43:THR:HG23 | 1.97                     | 0.63              |
| 28:DF:56:LEU:O     | 28:DF:59:ILE:HG22 | 1.97                     | 0.63              |
| 31:DJ:41:LYS:HG2   | 38:DQ:63:ARG:NH1  | 2.12                     | 0.63              |
| 37:DP:26:GLU:HA    | 37:DP:47:ILE:N    | 2.11                     | 0.63              |
| 37:DP:27:VAL:HG13  | 37:DP:47:ILE:CD1  | 2.26                     | 0.63              |
| 37:DP:27:VAL:CG1   | 37:DP:47:ILE:HD12 | 2.26                     | 0.63              |
| 42:DU:13:LEU:HD21  | 42:DU:69:VAL:HG13 | 1.79                     | 0.63              |
| 50:D3:4:LYS:HE3    | 50:D3:61:LEU:H    | 1.63                     | 0.63              |
| 6:AG:74:VAL:HG12   | 6:AG:75:LYS:H     | 1.62                     | 0.63              |
| 11:AL:20:VAL:O     | 11:AL:23:LEU:HG   | 1.97                     | 0.63              |
| 12:AM:88:LEU:O     | 12:AM:92:ARG:HG3  | 1.97                     | 0.63              |
| 21:AU:44:ARG:HH11  | 21:AU:44:ARG:HG3  | 1.64                     | 0.63              |
| 23:BB:41:C:H2'     | 23:BB:42:A:C8     | 2.33                     | 0.63              |
| 23:BB:364:C:H2'    | 23:BB:365:U:C6    | 2.33                     | 0.63              |
| 23:BB:828:U:H4'    | 23:BB:831:G:N1    | 2.13                     | 0.63              |
| 23:BB:1570:A:H2'   | 23:BB:1571:A:C8   | 2.34                     | 0.63              |
| 23:BB:1641:A:H2'   | 23:BB:1642:G:O4'  | 1.99                     | 0.63              |
| 26:BD:8:LYS:HB3    | 37:BP:5:LYS:HZ1   | 1.61                     | 0.63              |
| 27:BE:113:VAL:HG13 | 27:BE:114:ARG:H   | 1.63                     | 0.63              |
| 30:BH:6:LEU:HA     | 30:BH:15:LEU:C    | 2.23                     | 0.63              |
| 33:BL:90:VAL:CG1   | 33:BL:121:THR:H   | 2.10                     | 0.63              |
| 34:BM:67:VAL:HB    | 34:BM:100:LYS:HD3 | 1.79                     | 0.63              |
| 1:CA:390:U:H2'     | 1:CA:391:G:H8     | 1.62                     | 0.63              |
| 1:CA:947:G:H2'     | 1:CA:948:C:H6     | 1.63                     | 0.63              |
| 2:CC:53:ARG:HG3    | 2:CC:113:LYS:HD3  | 1.80                     | 0.63              |
| 8:CI:48:ARG:HA     | 8:CI:51:LEU:HD12  | 1.81                     | 0.63              |
| 20:CB:163:ILE:HG23 | 20:CB:164:ASP:N   | 2.13                     | 0.63              |
| 23:DB:598:U:H2'    | 23:DB:599:A:C8    | 2.34                     | 0.63              |
| 23:DB:608:A:H2'    | 23:DB:609:A:C8    | 2.34                     | 0.63              |
| 23:DB:1151:A:H2'   | 23:DB:1152:C:C6   | 2.33                     | 0.63              |
| 23:DB:1278:C:OP1   | 35:DN:36:THR:HG23 | 1.98                     | 0.63              |
| 26:DD:61:THR:HG23  | 26:DD:62:LYS:N    | 2.14                     | 0.63              |
| 32:DK:107:LEU:HD21 | 32:DK:115:ILE:CD1 | 2.28                     | 0.63              |
| 33:DL:78:ARG:HH12  | 33:DL:80:SER:HB3  | 1.63                     | 0.63              |
| 41:DT:21:SER:HA    | 41:DT:24:MET:SD   | 2.38                     | 0.63              |
| 42:DU:41:VAL:HA    | 42:DU:57:ILE:HD12 | 1.80                     | 0.63              |
| 1:AA:975:A:H5''    | 1:AA:976:G:O5'    | 1.99                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:AF:40:GLU:HG3   | 5:AF:42:TRP:HE1    | 1.64                     | 0.63              |
| 6:AG:65:LEU:O     | 6:AG:69:ARG:HG3    | 1.99                     | 0.63              |
| 15:AP:26:ASN:CG   | 15:AP:31:ARG:HB3   | 2.24                     | 0.63              |
| 20:AB:71:THR:HG22 | 20:AB:94:ARG:HH21  | 1.63                     | 0.63              |
| 22:BA:28:C:H5'    | 22:BA:29:A:OP2     | 1.98                     | 0.63              |
| 23:BB:1351:C:H4'  | 23:BB:1572:A:O4'   | 1.99                     | 0.63              |
| 23:BB:2784:U:H2'  | 23:BB:2785:C:C6    | 2.33                     | 0.63              |
| 27:BE:3:LEU:O     | 27:BE:4:VAL:HG12   | 1.98                     | 0.63              |
| 31:BJ:64:VAL:HG12 | 31:BJ:65:THR:H     | 1.64                     | 0.63              |
| 32:BK:11:ALA:HB3  | 32:BK:85:VAL:HG22  | 1.81                     | 0.63              |
| 1:CA:720:C:H4'    | 17:CR:38:ILE:HD11  | 1.81                     | 0.63              |
| 1:CA:1143:G:H2'   | 1:CA:1144:G:C8     | 2.34                     | 0.63              |
| 1:CA:1323:G:H2'   | 1:CA:1324:A:C8     | 2.34                     | 0.63              |
| 1:CA:1409:C:H2'   | 1:CA:1410:A:C8     | 2.33                     | 0.63              |
| 2:CC:149:LYS:HG3  | 2:CC:166:TRP:HE1   | 1.63                     | 0.63              |
| 7:CH:78:SER:HB2   | 7:CH:124:ILE:O     | 1.97                     | 0.63              |
| 7:CH:86:LYS:HD2   | 7:CH:90:GLU:HG2    | 1.81                     | 0.63              |
| 8:CI:54:VAL:HG12  | 8:CI:93:LEU:HD22   | 1.80                     | 0.63              |
| 23:DB:85:G:OP1    | 42:DU:4:ILE:HG23   | 1.98                     | 0.63              |
| 23:DB:143:C:N3    | 41:DT:3:ARG:NH1    | 2.46                     | 0.63              |
| 23:DB:1205:A:H62  | 27:DE:164:LEU:HD11 | 1.63                     | 0.63              |
| 23:DB:1854:A:H62  | 23:DB:1888:G:H8    | 1.46                     | 0.63              |
| 25:DC:86:ARG:C    | 25:DC:155:ARG:HH12 | 2.06                     | 0.63              |
| 26:DD:42:ASN:O    | 26:DD:43:ASP:HB2   | 1.97                     | 0.63              |
| 27:DE:2:GLU:HA    | 27:DE:16:GLU:HB3   | 1.81                     | 0.63              |
| 34:DM:97:GLN:N    | 34:DM:98:PRO:CD    | 2.61                     | 0.63              |
| 35:DN:79:LEU:HD22 | 35:DN:83:LEU:HD23  | 1.78                     | 0.63              |
| 37:DP:23:ASP:O    | 37:DP:25:VAL:N     | 2.32                     | 0.63              |
| 1:AA:74:A:H2'     | 1:AA:75:G:C5'      | 2.27                     | 0.63              |
| 1:AA:105:G:H2'    | 1:AA:106:C:H6      | 1.64                     | 0.63              |
| 1:AA:875:U:O2'    | 7:AH:14:ARG:HD2    | 1.97                     | 0.63              |
| 1:AA:1446:A:C2'   | 1:AA:1447:A:H5''   | 2.29                     | 0.63              |
| 3:AD:59:LYS:O     | 3:AD:63:ILE:HG13   | 1.98                     | 0.63              |
| 7:AH:11:THR:HG22  | 7:AH:15:ASN:ND2    | 2.13                     | 0.63              |
| 16:AQ:10:ARG:NH2  | 16:AQ:11:VAL:HG23  | 2.14                     | 0.63              |
| 23:BB:598:U:H2'   | 23:BB:599:A:C8     | 2.34                     | 0.63              |
| 23:BB:650:C:H5''  | 50:B3:22:LYS:NZ    | 2.13                     | 0.63              |
| 23:BB:813:U:H2'   | 23:BB:814:C:H6     | 1.62                     | 0.63              |
| 23:BB:967:U:H2'   | 23:BB:968:C:C6     | 2.33                     | 0.63              |
| 23:BB:1060:U:O4   | 23:BB:1088:A:N6    | 2.32                     | 0.63              |
| 23:BB:1509:A:H5'  | 23:BB:1510:G:H5'   | 1.80                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:1567:G:H5''  | 25:BC:84:PRO:HG3   | 1.81                     | 0.63              |
| 23:BB:2498:C:O2'   | 23:BB:2499:C:H5'   | 1.98                     | 0.63              |
| 23:BB:2852:G:H2'   | 23:BB:2853:C:C6    | 2.33                     | 0.63              |
| 24:BV:46:LYS:O     | 24:BV:50:MET:HG3   | 1.99                     | 0.63              |
| 24:BV:69:GLU:HG2   | 24:BV:70:ILE:N     | 2.14                     | 0.63              |
| 24:BV:89:ILE:HD12  | 24:BV:89:ILE:O     | 1.99                     | 0.63              |
| 25:BC:12:ARG:NE    | 25:BC:18:VAL:HG11  | 2.14                     | 0.63              |
| 25:BC:140:VAL:C    | 25:BC:193:GLU:HB2  | 2.23                     | 0.63              |
| 29:BG:86:LEU:HD13  | 29:BG:163:TYR:HA   | 1.79                     | 0.63              |
| 33:BL:38:GLN:O     | 33:BL:41:ARG:HD3   | 1.98                     | 0.63              |
| 35:BN:37:THR:HA    | 35:BN:109:PRO:O    | 1.98                     | 0.63              |
| 35:BN:113:ILE:HG22 | 35:BN:114:GLU:N    | 2.10                     | 0.63              |
| 36:BO:57:ALA:CB    | 36:BO:62:LEU:HD22  | 2.18                     | 0.63              |
| 37:BP:97:TYR:O     | 37:BP:98:TYR:HB2   | 1.97                     | 0.63              |
| 1:CA:1041:G:H2'    | 1:CA:1042:A:H8     | 1.64                     | 0.63              |
| 1:CA:1191:A:OP1    | 2:CC:2:GLN:HB2     | 1.98                     | 0.63              |
| 2:CC:52:SER:O      | 2:CC:53:ARG:HG3    | 1.98                     | 0.63              |
| 5:CF:79:ARG:NH2    | 5:CF:87:SER:HB3    | 2.14                     | 0.63              |
| 5:CF:86:ARG:NH1    | 17:CR:63:TYR:HB3   | 2.13                     | 0.63              |
| 13:CN:13:VAL:HG22  | 13:CN:59:GLN:NE2   | 2.14                     | 0.63              |
| 23:DB:64:A:H2'     | 23:DB:65:U:H6      | 1.64                     | 0.63              |
| 23:DB:365:U:H2'    | 23:DB:366:C:H6     | 1.61                     | 0.63              |
| 23:DB:532:A:N3     | 23:DB:532:A:H2'    | 2.13                     | 0.63              |
| 23:DB:1439:A:C6    | 23:DB:1552:A:N7    | 2.67                     | 0.63              |
| 23:DB:2498:C:O2'   | 23:DB:2499:C:H5'   | 1.99                     | 0.63              |
| 26:DD:9:VAL:HG12   | 26:DD:10:GLY:H     | 1.62                     | 0.63              |
| 31:DJ:77:HIS:HB2   | 31:DJ:85:LYS:HE2   | 1.81                     | 0.63              |
| 31:DJ:105:VAL:HG11 | 31:DJ:122:LEU:CD1  | 2.28                     | 0.63              |
| 32:DK:93:GLN:HG2   | 32:DK:94:PRO:HD2   | 1.79                     | 0.63              |
| 33:DL:126:ARG:HH12 | 33:DL:128:THR:HG22 | 1.64                     | 0.63              |
| 43:DW:67:LYS:HG2   | 43:DW:71:LYS:CB    | 2.29                     | 0.63              |
| 50:D3:24:LYS:NZ    | 50:D3:24:LYS:HB3   | 2.13                     | 0.63              |
| 1:AA:10:A:OP2      | 4:AE:130:THR:HB    | 1.98                     | 0.63              |
| 1:AA:1308:U:H2'    | 1:AA:1309:G:C8     | 2.33                     | 0.63              |
| 5:AF:53:LYS:CD     | 5:AF:54:LEU:H      | 2.10                     | 0.63              |
| 10:AK:58:THR:HG23  | 10:AK:61:ALA:HB2   | 1.80                     | 0.63              |
| 18:AS:28:LYS:HD3   | 18:AS:28:LYS:H     | 1.63                     | 0.63              |
| 23:BB:934:U:H2'    | 23:BB:935:C:H6     | 1.61                     | 0.63              |
| 27:BE:152:GLU:HG2  | 27:BE:171:ASP:HB3  | 1.80                     | 0.63              |
| 40:BS:47:VAL:HG12  | 40:BS:103:ILE:HD13 | 1.80                     | 0.63              |
| 43:BW:43:LYS:CG    | 43:BW:76:ARG:HE    | 2.12                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:32:A:H2'     | 1:CA:33:A:C8       | 2.34                     | 0.63              |
| 5:CF:3:HIS:CA     | 5:CF:65:GLU:HG3    | 2.28                     | 0.63              |
| 16:CQ:42:LYS:C    | 16:CQ:43:LEU:HD12  | 2.23                     | 0.63              |
| 20:CB:70:GLY:O    | 20:CB:92:ASN:HA    | 1.97                     | 0.63              |
| 23:DB:863:A:H2'   | 23:DB:864:G:C8     | 2.34                     | 0.63              |
| 23:DB:1351:C:H4'  | 23:DB:1572:A:O4'   | 1.99                     | 0.63              |
| 31:DJ:112:GLY:O   | 31:DJ:116:ARG:HB2  | 1.99                     | 0.63              |
| 33:DL:4:ASN:O     | 33:DL:5:THR:HG22   | 1.98                     | 0.63              |
| 35:DN:108:ALA:HB1 | 35:DN:109:PRO:HD2  | 1.81                     | 0.63              |
| 52:DI:5:GLN:HB2   | 52:DI:30:GLN:OE1   | 1.99                     | 0.63              |
| 1:AA:57:G:H2'     | 1:AA:58:C:H6       | 1.63                     | 0.63              |
| 1:AA:1254:A:OP1   | 9:AJ:47:GLU:HG3    | 1.99                     | 0.63              |
| 1:AA:1524:C:H2'   | 1:AA:1525:G:H8     | 1.63                     | 0.63              |
| 6:AG:87:PRO:HG2   | 6:AG:151:ALA:HB2   | 1.81                     | 0.63              |
| 13:AN:81:ILE:HD12 | 13:AN:82:LYS:H     | 1.64                     | 0.63              |
| 14:AO:60:SER:HA   | 14:AO:63:ARG:HH12  | 1.64                     | 0.63              |
| 18:AS:11:ASP:CG   | 18:AS:34:SER:HB2   | 2.23                     | 0.63              |
| 23:BB:38:A:O4'    | 27:BE:46:GLN:CG    | 2.40                     | 0.63              |
| 23:BB:263:G:H2'   | 23:BB:264:C:O4'    | 1.98                     | 0.63              |
| 23:BB:903:C:H2'   | 23:BB:904:G:H8     | 1.63                     | 0.63              |
| 23:BB:1439:A:C6   | 23:BB:1552:A:N7    | 2.67                     | 0.63              |
| 23:BB:1453:A:H61  | 35:BN:74:GLU:HG2   | 1.61                     | 0.63              |
| 26:BD:25:THR:HB   | 37:BP:5:LYS:NZ     | 2.13                     | 0.63              |
| 27:BE:48:THR:HA   | 27:BE:86:ALA:HB1   | 1.81                     | 0.63              |
| 34:BM:71:LYS:HE2  | 34:BM:91:TYR:C     | 2.23                     | 0.63              |
| 34:BM:101:VAL:C   | 34:BM:102:LEU:HD12 | 2.24                     | 0.63              |
| 38:BQ:57:ARG:HA   | 38:BQ:60:TRP:HE3   | 1.63                     | 0.63              |
| 42:BU:7:ASP:HA    | 42:BU:24:VAL:HA    | 1.81                     | 0.63              |
| 46:BZ:64:PHE:HA   | 46:BZ:67:PRO:HD2   | 1.81                     | 0.63              |
| 1:CA:976:G:OP1    | 13:CN:70:HIS:HA    | 1.98                     | 0.63              |
| 1:CA:1520:C:H2'   | 1:CA:1521:C:C6     | 2.34                     | 0.63              |
| 2:CC:52:SER:O     | 2:CC:113:LYS:HD3   | 1.99                     | 0.63              |
| 10:CK:124:LYS:CD  | 21:CU:34:ARG:HD3   | 2.28                     | 0.63              |
| 23:DB:181:A:H2'   | 23:DB:182:A:C8     | 2.33                     | 0.63              |
| 23:DB:283:G:H2'   | 23:DB:284:U:C6     | 2.34                     | 0.63              |
| 23:DB:1570:A:H2'  | 23:DB:1571:A:C8    | 2.34                     | 0.63              |
| 23:DB:1973:G:H2'  | 23:DB:1974:C:C6    | 2.33                     | 0.63              |
| 23:DB:2813:A:H2'  | 23:DB:2814:A:C8    | 2.34                     | 0.63              |
| 25:DC:19:VAL:HG12 | 25:DC:20:ASN:N     | 2.13                     | 0.63              |
| 33:DL:25:SER:C    | 33:DL:27:LEU:H     | 2.07                     | 0.63              |
| 49:D2:33:ARG:NE   | 49:D2:33:ARG:HA    | 2.13                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:168:G:O2'    | 1:AA:169:C:H5'     | 1.99                     | 0.63              |
| 1:AA:810:C:O2'    | 1:AA:811:C:H5'     | 1.99                     | 0.63              |
| 1:AA:1102:A:H2'   | 1:AA:1103:C:C6     | 2.34                     | 0.63              |
| 1:AA:1163:A:H2'   | 1:AA:1164:G:C8     | 2.34                     | 0.63              |
| 1:AA:1513:A:H2'   | 1:AA:1514:G:H8     | 1.63                     | 0.63              |
| 23:BB:41:C:H2'    | 23:BB:42:A:H8      | 1.63                     | 0.63              |
| 23:BB:588:U:OP1   | 33:BL:28:GLY:N     | 2.31                     | 0.63              |
| 23:BB:1309:G:H4'  | 49:B2:7:PRO:HG2    | 1.80                     | 0.63              |
| 23:BB:2212:A:N7   | 23:BB:2214:C:N4    | 2.46                     | 0.63              |
| 23:BB:2228:G:H2'  | 23:BB:2229:U:H6    | 1.63                     | 0.63              |
| 23:BB:2563:U:H5'' | 32:BK:27:GLY:HA2   | 1.79                     | 0.63              |
| 27:BE:3:LEU:HB2   | 27:BE:12:LEU:HD22  | 1.80                     | 0.63              |
| 29:BG:17:LYS:HE3  | 29:BG:24:THR:HG21  | 1.80                     | 0.63              |
| 30:BH:89:LYS:NZ   | 30:BH:123:ARG:HB3  | 2.13                     | 0.63              |
| 34:BM:3:GLN:O     | 34:BM:6:ARG:N      | 2.32                     | 0.63              |
| 34:BM:96:ILE:HD13 | 34:BM:97:GLN:HG3   | 1.80                     | 0.63              |
| 37:BP:91:VAL:HB   | 37:BP:113:LEU:HG   | 1.80                     | 0.63              |
| 40:BS:66:ILE:H    | 40:BS:66:ILE:HD12  | 1.64                     | 0.63              |
| 48:B1:35:LEU:C    | 48:B1:36:LYS:HD2   | 2.24                     | 0.63              |
| 49:B2:33:ARG:O    | 49:B2:37:LYS:HB2   | 1.98                     | 0.63              |
| 1:CA:57:G:H2'     | 1:CA:58:C:H6       | 1.63                     | 0.63              |
| 1:CA:763:G:H2'    | 1:CA:764:C:C6      | 2.34                     | 0.63              |
| 1:CA:1234:C:H2'   | 1:CA:1235:U:C6     | 2.34                     | 0.63              |
| 1:CA:1342:C:H2'   | 1:CA:1343:G:H8     | 1.64                     | 0.63              |
| 13:CN:19:TYR:HE2  | 13:CN:50:LEU:HD13  | 1.64                     | 0.63              |
| 22:DA:43:C:H4'    | 28:DF:62:GLN:HE21  | 1.64                     | 0.63              |
| 23:DB:631:A:O2'   | 33:DL:66:PHE:HB3   | 1.98                     | 0.63              |
| 23:DB:782:A:O2'   | 25:DC:223:ALA:HB1  | 1.98                     | 0.63              |
| 23:DB:1022:G:C8   | 31:DJ:68:LYS:HE3   | 2.34                     | 0.63              |
| 23:DB:1174:U:H1'  | 23:DB:1176:U:C4    | 2.34                     | 0.63              |
| 23:DB:1548:A:H2'  | 23:DB:1549:A:H8    | 1.63                     | 0.63              |
| 25:DC:16:VAL:HG12 | 25:DC:16:VAL:O     | 1.97                     | 0.63              |
| 25:DC:19:VAL:HB   | 25:DC:205:GLY:HA2  | 1.80                     | 0.63              |
| 31:DJ:69:ARG:HH11 | 31:DJ:69:ARG:HG3   | 1.62                     | 0.63              |
| 35:DN:45:ARG:NH2  | 35:DN:113:ILE:HD12 | 2.12                     | 0.63              |
| 50:D3:4:LYS:HG3   | 50:D3:61:LEU:HB2   | 1.81                     | 0.63              |
| 1:AA:278:G:N2     | 1:AA:279:A:H62     | 1.97                     | 0.62              |
| 12:AM:22:TYR:HB3  | 12:AM:69:ARG:HH22  | 1.63                     | 0.62              |
| 23:BB:65:U:H2'    | 23:BB:66:C:H6      | 1.64                     | 0.62              |
| 23:BB:608:A:H2'   | 23:BB:609:A:C8     | 2.34                     | 0.62              |
| 23:BB:856:G:H2'   | 23:BB:857:G:C8     | 2.34                     | 0.62              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:1158:C:H5''  | 45:BY:30:ARG:HD3   | 1.81                     | 0.62              |
| 23:BB:1386:C:H2'   | 23:BB:1387:A:C8    | 2.34                     | 0.62              |
| 23:BB:1442:U:H2'   | 23:BB:1443:U:C6    | 2.33                     | 0.62              |
| 23:BB:1854:A:H62   | 23:BB:1888:G:H8    | 1.46                     | 0.62              |
| 23:BB:2415:G:H2'   | 23:BB:2416:C:H6    | 1.62                     | 0.62              |
| 26:BD:115:GLY:HA3  | 26:BD:166:GLY:HA2  | 1.80                     | 0.62              |
| 32:BK:99:ILE:HD13  | 32:BK:118:LEU:HD13 | 1.80                     | 0.62              |
| 34:BM:34:LYS:O     | 34:BM:124:LEU:HB2  | 1.99                     | 0.62              |
| 37:BP:63:ILE:HD12  | 37:BP:63:ILE:H     | 1.64                     | 0.62              |
| 42:BU:27:VAL:HA    | 42:BU:32:LYS:O     | 1.99                     | 0.62              |
| 2:CC:61:LYS:HB3    | 2:CC:61:LYS:NZ     | 2.14                     | 0.62              |
| 2:CC:182:ASP:HB3   | 2:CC:201:ILE:HB    | 1.80                     | 0.62              |
| 5:CF:38:ARG:HH21   | 5:CF:63:ASN:HD21   | 1.46                     | 0.62              |
| 16:CQ:11:VAL:HG22  | 16:CQ:22:VAL:HG22  | 1.81                     | 0.62              |
| 20:CB:65:LYS:HB2   | 20:CB:157:PRO:HA   | 1.80                     | 0.62              |
| 23:DB:6:A:H2'      | 23:DB:7:G:C8       | 2.34                     | 0.62              |
| 23:DB:967:U:H2'    | 23:DB:968:C:C6     | 2.34                     | 0.62              |
| 23:DB:1548:A:H2'   | 23:DB:1549:A:C8    | 2.34                     | 0.62              |
| 23:DB:1571:A:H2'   | 23:DB:1572:A:C8    | 2.34                     | 0.62              |
| 23:DB:1682:G:H2'   | 23:DB:1683:U:C6    | 2.34                     | 0.62              |
| 23:DB:1722:A:H2'   | 23:DB:1723:G:C8    | 2.34                     | 0.62              |
| 25:DC:131:MET:HG3  | 25:DC:187:CYS:SG   | 2.39                     | 0.62              |
| 29:DG:168:VAL:HG23 | 51:D4:31:PRO:HB3   | 1.81                     | 0.62              |
| 34:DM:18:ARG:H     | 34:DM:18:ARG:CD    | 2.09                     | 0.62              |
| 37:DP:89:GLY:HA2   | 37:DP:112:ARG:HH22 | 1.64                     | 0.62              |
| 52:DI:20:SER:O     | 52:DI:25:PRO:HD2   | 1.99                     | 0.62              |
| 52:DI:45:THR:CA    | 52:DI:48:ILE:HG22  | 2.29                     | 0.62              |
| 1:AA:1074:G:H2'    | 1:AA:1075:U:H6     | 1.64                     | 0.62              |
| 10:AK:58:THR:HG23  | 10:AK:61:ALA:CB    | 2.30                     | 0.62              |
| 16:AQ:10:ARG:HH11  | 16:AQ:55:GLY:N     | 1.96                     | 0.62              |
| 23:BB:381:G:O2'    | 23:BB:382:A:H5'    | 1.99                     | 0.62              |
| 23:BB:444:C:H5''   | 27:BE:44:ARG:NH1   | 2.14                     | 0.62              |
| 23:BB:547:A:H3'    | 23:BB:548:G:C8     | 2.28                     | 0.62              |
| 23:BB:1590:A:H2'   | 23:BB:1591:A:H8    | 1.64                     | 0.62              |
| 23:BB:2227:A:H4'   | 25:BC:258:SER:HA   | 1.80                     | 0.62              |
| 23:BB:2574:G:O2'   | 26:BD:151:THR:HG21 | 1.99                     | 0.62              |
| 25:BC:245:THR:O    | 25:BC:247:TRP:N    | 2.32                     | 0.62              |
| 28:BF:128:SER:HA   | 28:BF:154:THR:HG23 | 1.81                     | 0.62              |
| 29:BG:158:GLY:HA3  | 29:BG:170:THR:HG21 | 1.80                     | 0.62              |
| 39:BR:41:ILE:O     | 39:BR:43:ASN:N     | 2.31                     | 0.62              |
| 39:BR:78:ARG:HD3   | 39:BR:88:GLY:N     | 2.14                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 44:BX:43:LEU:HA   | 44:BX:47:ARG:HB3   | 1.81                     | 0.62              |
| 49:B2:35:ARG:HH12 | 49:B2:39:ARG:HG2   | 1.63                     | 0.62              |
| 1:CA:524:G:H2'    | 1:CA:525:C:C6      | 2.34                     | 0.62              |
| 1:CA:939:G:H5''   | 6:CG:101:ARG:HH22  | 1.63                     | 0.62              |
| 1:CA:1250:A:C4'   | 8:CI:69:GLY:H      | 2.10                     | 0.62              |
| 8:CI:29:ILE:HG23  | 8:CI:32:ARG:HB2    | 1.81                     | 0.62              |
| 10:CK:69:CYS:C    | 10:CK:73:VAL:HG22  | 2.24                     | 0.62              |
| 23:DB:1060:U:O4   | 23:DB:1088:A:N6    | 2.31                     | 0.62              |
| 23:DB:1386:C:H2'  | 23:DB:1387:A:C8    | 2.34                     | 0.62              |
| 23:DB:2742:G:H5'' | 51:D4:38:GLY:HA2   | 1.80                     | 0.62              |
| 23:DB:2848:G:H1'  | 23:DB:2868:A:N6    | 2.14                     | 0.62              |
| 25:DC:10:PRO:CD   | 25:DC:202:ARG:HH22 | 2.12                     | 0.62              |
| 27:DE:189:THR:C   | 27:DE:191:ASP:H    | 2.06                     | 0.62              |
| 32:DK:43:ILE:HG12 | 32:DK:52:VAL:HG12  | 1.81                     | 0.62              |
| 32:DK:66:LYS:HA   | 32:DK:79:PHE:O     | 1.99                     | 0.62              |
| 33:DL:2:ARG:HH11  | 33:DL:2:ARG:HG3    | 1.64                     | 0.62              |
| 35:DN:11:ASN:C    | 35:DN:12:ARG:HD3   | 2.24                     | 0.62              |
| 36:DO:91:SER:HB3  | 36:DO:115:LEU:HD22 | 1.81                     | 0.62              |
| 37:DP:91:VAL:HG23 | 37:DP:92:ARG:H     | 1.65                     | 0.62              |
| 40:DS:27:LYS:HA   | 40:DS:70:LYS:HB3   | 1.81                     | 0.62              |
| 42:DU:79:ALA:O    | 42:DU:96:LYS:HB3   | 1.99                     | 0.62              |
| 44:DX:50:VAL:O    | 44:DX:54:LYS:HB2   | 1.99                     | 0.62              |
| 1:AA:408:A:H3'    | 1:AA:409:U:H6      | 1.63                     | 0.62              |
| 1:AA:636:U:H2'    | 1:AA:637:C:C6      | 2.35                     | 0.62              |
| 3:AD:123:MET:HE3  | 3:AD:126:GLY:HA2   | 1.81                     | 0.62              |
| 9:AJ:30:LYS:HB2   | 9:AJ:36:VAL:HG21   | 1.81                     | 0.62              |
| 12:AM:89:ARG:HB2  | 12:AM:96:VAL:HG12  | 1.81                     | 0.62              |
| 13:AN:63:CYS:HB3  | 13:AN:67:GLY:N     | 2.08                     | 0.62              |
| 23:BB:244:A:H2'   | 23:BB:245:G:O4'    | 2.00                     | 0.62              |
| 23:BB:1319:C:O2'  | 23:BB:1320:C:H5'   | 1.98                     | 0.62              |
| 23:BB:1779:U:H5   | 23:BB:1784:A:N7    | 1.97                     | 0.62              |
| 23:BB:2274:A:H2'  | 23:BB:2276:G:OP1   | 2.00                     | 0.62              |
| 23:BB:2575:C:C4'  | 26:BD:148:GLN:HA   | 2.28                     | 0.62              |
| 25:BC:46:GLY:O    | 25:BC:47:ARG:HB2   | 1.98                     | 0.62              |
| 25:BC:224:MET:HA  | 25:BC:232:GLY:CA   | 2.28                     | 0.62              |
| 26:BD:4:LEU:HD13  | 26:BD:79:LEU:CD1   | 2.28                     | 0.62              |
| 26:BD:46:ARG:HD2  | 26:BD:80:TRP:CZ2   | 2.34                     | 0.62              |
| 29:BG:136:ASP:OD1 | 29:BG:138:GLN:HB3  | 1.99                     | 0.62              |
| 43:BW:42:THR:HA   | 43:BW:74:LYS:HA    | 1.80                     | 0.62              |
| 44:BX:28:LEU:HB3  | 44:BX:34:SER:CA    | 2.24                     | 0.62              |
| 3:CD:148:ALA:O    | 3:CD:151:GLN:HG2   | 1.99                     | 0.62              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:CH:35:ILE:O      | 7:CH:38:VAL:HG12  | 1.99                     | 0.62              |
| 23:DB:182:A:H2'    | 23:DB:183:C:H6    | 1.63                     | 0.62              |
| 23:DB:1024:G:C3'   | 23:DB:1025:G:H5'' | 2.28                     | 0.62              |
| 23:DB:1100:C:H2'   | 23:DB:1101:U:H6   | 1.64                     | 0.62              |
| 23:DB:1365:A:OP2   | 46:DZ:9:TYR:HE2   | 1.81                     | 0.62              |
| 23:DB:1802:A:H2'   | 23:DB:1803:A:C8   | 2.34                     | 0.62              |
| 23:DB:2306:C:H3'   | 23:DB:2307:G:C5'  | 2.29                     | 0.62              |
| 23:DB:2415:G:H2'   | 23:DB:2416:C:H6   | 1.62                     | 0.62              |
| 25:DC:3:VAL:HG12   | 25:DC:4:LYS:H     | 1.64                     | 0.62              |
| 26:DD:125:TRP:CD1  | 26:DD:127:PHE:HB2 | 2.34                     | 0.62              |
| 35:DN:87:PHE:CD1   | 35:DN:90:ARG:HB2  | 2.34                     | 0.62              |
| 43:DW:35:ILE:H     | 43:DW:35:ILE:CD1  | 2.10                     | 0.62              |
| 1:AA:918:A:H2'     | 1:AA:919:A:C8     | 2.34                     | 0.62              |
| 8:AI:11:ARG:NH2    | 8:AI:12:LYS:HB2   | 2.14                     | 0.62              |
| 10:AK:22:ILE:HD13  | 10:AK:95:THR:HG21 | 1.81                     | 0.62              |
| 10:AK:56:LYS:HD3   | 10:AK:56:LYS:H    | 1.64                     | 0.62              |
| 12:AM:67:ASP:CG    | 28:BF:111:ARG:HB3 | 2.25                     | 0.62              |
| 15:AP:71:VAL:HA    | 15:AP:74:LEU:HG   | 1.79                     | 0.62              |
| 23:BB:143:C:H2'    | 23:BB:144:A:N9    | 2.13                     | 0.62              |
| 23:BB:172:A:H2'    | 23:BB:173:A:C8    | 2.34                     | 0.62              |
| 23:BB:932:U:H5'    | 23:BB:933:A:OP1   | 1.99                     | 0.62              |
| 23:BB:1097:U:H2'   | 23:BB:1098:A:H5'  | 1.81                     | 0.62              |
| 23:BB:1131:G:H1'   | 23:BB:1133:A:N6   | 2.14                     | 0.62              |
| 25:BC:63:ILE:HG22  | 25:BC:64:VAL:H    | 1.64                     | 0.62              |
| 27:BE:109:LEU:HD23 | 27:BE:110:SER:N   | 2.14                     | 0.62              |
| 34:BM:45:GLN:NE2   | 34:BM:119:LEU:HB3 | 2.14                     | 0.62              |
| 34:BM:71:LYS:HD2   | 34:BM:71:LYS:C    | 2.24                     | 0.62              |
| 44:BX:30:MET:HG3   | 44:BX:31:GLN:N    | 2.14                     | 0.62              |
| 1:CA:636:U:H2'     | 1:CA:637:C:C6     | 2.34                     | 0.62              |
| 12:CM:56:ARG:HH11  | 12:CM:56:ARG:HG3  | 1.63                     | 0.62              |
| 23:DB:1295:C:H2'   | 23:DB:1296:G:H8   | 1.64                     | 0.62              |
| 23:DB:2088:A:H2'   | 23:DB:2089:C:H6   | 1.64                     | 0.62              |
| 23:DB:2292:U:H2'   | 23:DB:2293:G:C8   | 2.34                     | 0.62              |
| 30:DH:65:ALA:HA    | 30:DH:68:ARG:HB2  | 1.81                     | 0.62              |
| 34:DM:16:ARG:HH22  | 34:DM:72:PRO:HG2  | 1.65                     | 0.62              |
| 36:DO:51:ALA:HB3   | 36:DO:78:VAL:HG22 | 1.81                     | 0.62              |
| 36:DO:71:ALA:HB1   | 36:DO:106:LEU:HB2 | 1.81                     | 0.62              |
| 38:DQ:92:LYS:C     | 38:DQ:94:LEU:H    | 2.07                     | 0.62              |
| 39:DR:39:LEU:H     | 39:DR:61:ALA:CB   | 2.11                     | 0.62              |
| 43:DW:13:ARG:HE    | 43:DW:13:ARG:N    | 1.88                     | 0.62              |
| 52:DI:71:LYS:HB3   | 52:DI:115:ASP:OD2 | 1.99                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:AE:84:VAL:HG22   | 4:AE:85:LYS:H     | 1.65                     | 0.62              |
| 13:AN:42:ASN:O     | 13:AN:46:LYS:HG3  | 2.00                     | 0.62              |
| 23:BB:19:A:H5''    | 38:BQ:20:ALA:O    | 1.99                     | 0.62              |
| 23:BB:479:A:O2'    | 23:BB:480:A:OP2   | 2.15                     | 0.62              |
| 23:BB:969:G:H2'    | 23:BB:970:U:C6    | 2.35                     | 0.62              |
| 23:BB:1485:U:H2'   | 23:BB:1486:U:H6   | 1.63                     | 0.62              |
| 23:BB:1548:A:H2'   | 23:BB:1549:A:C8   | 2.34                     | 0.62              |
| 23:BB:1818:U:O3'   | 25:BC:155:ARG:HB2 | 2.00                     | 0.62              |
| 23:BB:2282:G:O2'   | 23:BB:2283:C:OP2  | 2.15                     | 0.62              |
| 26:BD:62:LYS:HG2   | 26:BD:63:PRO:CD   | 2.29                     | 0.62              |
| 33:BL:79:LEU:H     | 33:BL:79:LEU:HD12 | 1.64                     | 0.62              |
| 34:BM:65:ILE:HG22  | 34:BM:101:VAL:HA  | 1.82                     | 0.62              |
| 1:CA:107:G:H2'     | 1:CA:108:G:H5''   | 1.81                     | 0.62              |
| 1:CA:492:C:C2'     | 1:CA:493:A:H5''   | 2.28                     | 0.62              |
| 1:CA:980:C:H2'     | 1:CA:981:U:H5'    | 1.80                     | 0.62              |
| 1:CA:1071:C:H2'    | 1:CA:1072:G:C8    | 2.33                     | 0.62              |
| 1:CA:1329:A:H5''   | 12:CM:25:GLY:H    | 1.63                     | 0.62              |
| 4:CE:95:MET:HA     | 4:CE:124:ALA:HB2  | 1.79                     | 0.62              |
| 7:CH:19:ALA:HB3    | 7:CH:21:LYS:HG2   | 1.80                     | 0.62              |
| 16:CQ:24:ILE:HD13  | 16:CQ:43:LEU:HD13 | 1.81                     | 0.62              |
| 23:DB:438:G:H2'    | 23:DB:439:A:C8    | 2.34                     | 0.62              |
| 23:DB:1098:A:O5'   | 52:DI:3:LYS:HG2   | 2.00                     | 0.62              |
| 23:DB:1117:C:O4'   | 34:DM:136:MET:HE1 | 1.99                     | 0.62              |
| 23:DB:1590:A:H2'   | 23:DB:1591:A:H8   | 1.64                     | 0.62              |
| 23:DB:2233:U:H2'   | 23:DB:2234:G:C8   | 2.35                     | 0.62              |
| 25:DC:21:PRO:HD2   | 25:DC:202:ARG:NH1 | 2.13                     | 0.62              |
| 25:DC:28:PRO:HB2   | 25:DC:79:ARG:HG2  | 1.80                     | 0.62              |
| 25:DC:235:GLU:HG3  | 25:DC:236:GLY:H   | 1.64                     | 0.62              |
| 29:DG:75:VAL:O     | 29:DG:79:THR:HG22 | 1.99                     | 0.62              |
| 37:DP:69:VAL:HG13  | 37:DP:70:GLU:N    | 2.12                     | 0.62              |
| 50:D3:4:LYS:HE3    | 50:D3:61:LEU:HB2  | 1.81                     | 0.62              |
| 1:AA:957:U:H3      | 1:AA:960:U:H5''   | 1.65                     | 0.62              |
| 3:AD:147:LYS:H     | 3:AD:147:LYS:HE3  | 1.65                     | 0.62              |
| 20:AB:75:ALA:O     | 20:AB:79:VAL:HB   | 2.00                     | 0.62              |
| 20:AB:101:THR:HG23 | 20:AB:102:ASN:H   | 1.65                     | 0.62              |
| 23:BB:274:C:H2'    | 23:BB:275:C:O4'   | 2.00                     | 0.62              |
| 23:BB:536:G:H4'    | 38:BQ:56:PHE:CZ   | 2.35                     | 0.62              |
| 23:BB:2066:C:O2'   | 23:BB:2067:G:H5'  | 2.00                     | 0.62              |
| 23:BB:2678:C:H2'   | 23:BB:2679:A:C8   | 2.35                     | 0.62              |
| 23:BB:2848:G:H1'   | 23:BB:2868:A:N6   | 2.14                     | 0.62              |
| 25:BC:220:ARG:CZ   | 25:BC:220:ARG:HA  | 2.29                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:BD:107:VAL:HG23 | 26:BD:204:LYS:O    | 2.00                     | 0.62              |
| 30:BH:82:SER:HB2   | 30:BH:94:ILE:HD11  | 1.80                     | 0.62              |
| 38:BQ:101:ASP:HB3  | 38:BQ:104:ALA:HB3  | 1.81                     | 0.62              |
| 40:BS:4:ILE:HG22   | 40:BS:5:ALA:H      | 1.64                     | 0.62              |
| 41:BT:3:ARG:HD3    | 41:BT:3:ARG:C      | 2.23                     | 0.62              |
| 1:CA:384:G:H2'     | 1:CA:385:C:C6      | 2.34                     | 0.62              |
| 1:CA:810:C:O2'     | 1:CA:811:C:H5'     | 1.99                     | 0.62              |
| 1:CA:1143:G:H2'    | 1:CA:1144:G:H8     | 1.64                     | 0.62              |
| 1:CA:1392:G:O2'    | 1:CA:1393:U:H5'    | 2.00                     | 0.62              |
| 1:CA:1409:C:H2'    | 1:CA:1410:A:H8     | 1.65                     | 0.62              |
| 9:CJ:53:ILE:HG22   | 9:CJ:61:ALA:HB1    | 1.81                     | 0.62              |
| 13:CN:32:ASP:HB2   | 13:CN:34:ASN:ND2   | 2.14                     | 0.62              |
| 15:CP:20:VAL:HG23  | 15:CP:34:GLU:O     | 1.99                     | 0.62              |
| 20:CB:162:VAL:HG11 | 20:CB:172:ILE:HD11 | 1.82                     | 0.62              |
| 23:DB:340:A:H2'    | 23:DB:341:C:O4'    | 1.99                     | 0.62              |
| 23:DB:997:G:H5'    | 38:DQ:92:LYS:HG3   | 1.81                     | 0.62              |
| 23:DB:1099:G:C8    | 52:DI:3:LYS:CB     | 2.83                     | 0.62              |
| 23:DB:1151:A:H2'   | 23:DB:1152:C:H6    | 1.63                     | 0.62              |
| 23:DB:1459:G:O2'   | 23:DB:1460:U:H5'   | 1.98                     | 0.62              |
| 25:DC:68:ARG:NH2   | 25:DC:190:THR:HG23 | 2.14                     | 0.62              |
| 27:DE:191:ASP:HA   | 27:DE:194:LYS:HE3  | 1.81                     | 0.62              |
| 30:DH:96:THR:HG23  | 30:DH:97:ARG:HG2   | 1.81                     | 0.62              |
| 42:DU:23:LYS:C     | 42:DU:25:LYS:HD2   | 2.24                     | 0.62              |
| 1:AA:973:G:H1'     | 9:AJ:56:HIS:ND1    | 2.15                     | 0.62              |
| 1:AA:1017:U:H2'    | 1:AA:1018:G:C8     | 2.34                     | 0.62              |
| 3:AD:20:LEU:O      | 3:AD:21:LYS:HE3    | 2.00                     | 0.62              |
| 9:AJ:24:GLU:OE1    | 9:AJ:90:LEU:HD22   | 1.98                     | 0.62              |
| 20:AB:128:LEU:HG   | 20:AB:132:GLU:HG2  | 1.82                     | 0.62              |
| 23:BB:364:C:H2'    | 23:BB:365:U:H6     | 1.65                     | 0.62              |
| 23:BB:633:A:H2'    | 23:BB:634:C:H5'    | 1.81                     | 0.62              |
| 23:BB:1155:A:H61   | 45:BY:10:ARG:HH12  | 1.46                     | 0.62              |
| 23:BB:1571:A:H2'   | 23:BB:1572:A:C8    | 2.34                     | 0.62              |
| 23:BB:1843:C:H5''  | 25:BC:252:LYS:NZ   | 2.15                     | 0.62              |
| 23:BB:2813:A:H2'   | 23:BB:2814:A:C8    | 2.34                     | 0.62              |
| 25:BC:107:LYS:H    | 25:BC:194:VAL:HG21 | 1.63                     | 0.62              |
| 28:BF:33:ILE:HD11  | 28:BF:90:LEU:HB2   | 1.81                     | 0.62              |
| 36:BO:1:MET:HG2    | 36:BO:3:LYS:N      | 2.15                     | 0.62              |
| 37:BP:86:LYS:O     | 37:BP:87:ARG:HG3   | 1.99                     | 0.62              |
| 44:BX:29:ARG:HA    | 44:BX:34:SER:HB2   | 1.82                     | 0.62              |
| 5:CF:47:LEU:HD21   | 5:CF:57:ALA:CB     | 2.30                     | 0.62              |
| 23:DB:28:A:N6      | 23:DB:512:G:H1'    | 2.14                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:337:C:H2'    | 23:DB:338:G:O4'    | 1.99                     | 0.62              |
| 23:DB:1098:A:C3'   | 52:DI:4:VAL:N      | 2.62                     | 0.62              |
| 23:DB:1495:A:H2'   | 23:DB:1496:A:C8    | 2.35                     | 0.62              |
| 23:DB:2249:U:H4'   | 23:DB:2275:C:H5    | 1.65                     | 0.62              |
| 26:DD:17:GLU:HG2   | 37:DP:80:VAL:HB    | 1.81                     | 0.62              |
| 26:DD:30:GLU:HG2   | 26:DD:94:GLN:HE22  | 1.64                     | 0.62              |
| 32:DK:33:ALA:HB2   | 32:DK:39:ILE:HD11  | 1.81                     | 0.62              |
| 33:DL:118:THR:O    | 33:DL:119:PRO:C    | 2.39                     | 0.62              |
| 33:DL:118:THR:HG23 | 33:DL:119:PRO:CD   | 2.29                     | 0.62              |
| 34:DM:41:LEU:HD23  | 34:DM:93:VAL:HG11  | 1.82                     | 0.62              |
| 39:DR:6:GLN:NE2    | 39:DR:6:GLN:N      | 2.47                     | 0.62              |
| 40:DS:7:HIS:CD2    | 40:DS:10:ALA:HB2   | 2.35                     | 0.62              |
| 42:DU:46:LYS:HD3   | 42:DU:53:GLN:HG3   | 1.82                     | 0.62              |
| 42:DU:71:ILE:HG21  | 42:DU:102:ILE:HD12 | 1.80                     | 0.62              |
| 43:DW:35:ILE:HB    | 43:DW:67:LYS:HZ2   | 1.64                     | 0.62              |
| 47:D0:41:HIS:CD2   | 47:D0:46:GLY:HA2   | 2.35                     | 0.62              |
| 1:AA:135:C:O2      | 15:AP:1:MET:HB2    | 1.99                     | 0.62              |
| 1:AA:763:G:H2'     | 1:AA:764:C:C6      | 2.33                     | 0.62              |
| 1:AA:841:C:H3'     | 1:AA:843:U:OP2     | 1.99                     | 0.62              |
| 1:AA:1005:A:H3'    | 1:AA:1006:G:H8     | 1.64                     | 0.62              |
| 1:AA:1444:U:H2'    | 1:AA:1445:U:C6     | 2.35                     | 0.62              |
| 12:AM:48:SER:O     | 12:AM:52:ILE:HG22  | 1.98                     | 0.62              |
| 20:AB:147:LEU:O    | 20:AB:150:ILE:HG22 | 2.00                     | 0.62              |
| 23:BB:162:U:O2'    | 23:BB:163:C:H5'    | 2.00                     | 0.62              |
| 23:BB:365:U:H2'    | 23:BB:366:C:C6     | 2.35                     | 0.62              |
| 23:BB:968:C:H2'    | 23:BB:969:G:H8     | 1.64                     | 0.62              |
| 23:BB:1469:A:H2'   | 23:BB:1470:A:H8    | 1.62                     | 0.62              |
| 25:BC:67:LYS:O     | 25:BC:68:ARG:HB2   | 1.99                     | 0.62              |
| 28:BF:116:LEU:HG   | 28:BF:176:PHE:HA   | 1.80                     | 0.62              |
| 28:BF:177:ARG:HE   | 28:BF:178:LYS:N    | 1.97                     | 0.62              |
| 32:BK:35:VAL:HG12  | 32:BK:69:VAL:HG22  | 1.82                     | 0.62              |
| 33:BL:94:THR:CB    | 33:BL:103:ILE:HG12 | 2.29                     | 0.62              |
| 37:BP:52:ARG:HH11  | 37:BP:54:LEU:HB3   | 1.63                     | 0.62              |
| 38:BQ:111:LYS:HB2  | 39:BR:52:PRO:HB3   | 1.82                     | 0.62              |
| 41:BT:6:ARG:O      | 41:BT:6:ARG:HG3    | 1.97                     | 0.62              |
| 43:BW:35:ILE:HG23  | 43:BW:36:ILE:N     | 2.11                     | 0.62              |
| 9:CJ:85:ASP:HB2    | 9:CJ:89:ARG:NH2    | 2.14                     | 0.62              |
| 20:CB:46:VAL:HA    | 20:CB:49:PHE:CD2   | 2.35                     | 0.62              |
| 23:DB:1178:C:H2'   | 23:DB:1179:G:H8    | 1.63                     | 0.62              |
| 23:DB:2147:A:H4'   | 23:DB:2148:G:C8    | 2.34                     | 0.62              |
| 23:DB:2784:U:H2'   | 23:DB:2785:C:H6    | 1.62                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:DD:31:ALA:HB3   | 26:DD:95:SER:H     | 1.65                     | 0.62              |
| 27:DE:134:LEU:HD13 | 27:DE:134:LEU:H    | 1.65                     | 0.62              |
| 35:DN:30:ARG:HH12  | 35:DN:74:GLU:HG2   | 1.63                     | 0.62              |
| 39:DR:69:GLY:HA2   | 39:DR:96:VAL:HA    | 1.81                     | 0.62              |
| 42:DU:57:ILE:HD13  | 42:DU:58:VAL:N     | 2.13                     | 0.62              |
| 1:AA:107:G:H2'     | 1:AA:108:G:H5''    | 1.81                     | 0.62              |
| 3:AD:163:GLN:HB2   | 3:AD:164:ARG:NH1   | 2.14                     | 0.62              |
| 10:AK:105:ARG:HH21 | 21:AU:10:PRO:HG3   | 1.64                     | 0.62              |
| 13:AN:17:ASP:HA    | 13:AN:21:ALA:CB    | 2.30                     | 0.62              |
| 20:AB:66:ILE:C     | 20:AB:67:LEU:HD13  | 2.25                     | 0.62              |
| 20:AB:156:LEU:H    | 20:AB:156:LEU:HD12 | 1.63                     | 0.62              |
| 23:BB:854:C:H2'    | 23:BB:855:G:H8     | 1.65                     | 0.62              |
| 23:BB:923:G:O2'    | 23:BB:924:G:H5'    | 2.00                     | 0.62              |
| 23:BB:1159:U:H2'   | 23:BB:1160:G:H8    | 1.63                     | 0.62              |
| 23:BB:1802:A:H2'   | 23:BB:1803:A:C8    | 2.34                     | 0.62              |
| 23:BB:2185:U:H2'   | 23:BB:2186:G:H8    | 1.64                     | 0.62              |
| 23:BB:2678:C:H2'   | 23:BB:2679:A:H8    | 1.65                     | 0.62              |
| 26:BD:32:ASN:ND2   | 26:BD:94:GLN:HG2   | 2.15                     | 0.62              |
| 26:BD:106:LYS:HZ1  | 26:BD:208:LYS:HD3  | 1.65                     | 0.62              |
| 27:BE:24:ASN:CG    | 27:BE:24:ASN:O     | 2.43                     | 0.62              |
| 27:BE:147:LEU:HB3  | 27:BE:183:PHE:CD2  | 2.35                     | 0.62              |
| 29:BG:71:LEU:HA    | 29:BG:74:MET:HG3   | 1.82                     | 0.62              |
| 31:BJ:67:ASN:O     | 31:BJ:70:THR:HG22  | 1.99                     | 0.62              |
| 33:BL:79:LEU:HD12  | 33:BL:79:LEU:N     | 2.15                     | 0.62              |
| 34:BM:3:GLN:NE2    | 34:BM:5:LYS:H      | 1.98                     | 0.62              |
| 38:BQ:60:TRP:O     | 38:BQ:64:ILE:HG13  | 2.00                     | 0.62              |
| 43:BW:44:PHE:CE2   | 43:BW:60:ALA:HB3   | 2.34                     | 0.62              |
| 51:B4:2:LYS:NZ     | 51:B4:2:LYS:HB3    | 2.15                     | 0.62              |
| 1:CA:408:A:H3'     | 1:CA:409:U:H6      | 1.63                     | 0.62              |
| 1:CA:1354:U:H2'    | 1:CA:1355:G:H8     | 1.63                     | 0.62              |
| 6:CG:30:MET:HG3    | 6:CG:34:LYS:O      | 2.00                     | 0.62              |
| 6:CG:59:GLU:HA     | 6:CG:62:GLU:OE2    | 1.99                     | 0.62              |
| 8:CI:94:ARG:HB3    | 8:CI:98:ARG:NE     | 2.14                     | 0.62              |
| 23:DB:1509:A:H5'   | 23:DB:1510:G:H5'   | 1.80                     | 0.62              |
| 23:DB:1551:A:C3'   | 23:DB:1552:A:H5''  | 2.30                     | 0.62              |
| 23:DB:1641:A:H2'   | 23:DB:1642:G:O4'   | 1.98                     | 0.62              |
| 25:DC:139:THR:HA   | 25:DC:193:GLU:OE1  | 2.00                     | 0.62              |
| 34:DM:26:VAL:HG12  | 34:DM:27:SER:H     | 1.64                     | 0.62              |
| 35:DN:70:THR:HG22  | 35:DN:72:ASP:H     | 1.65                     | 0.62              |
| 1:AA:313:A:H2'     | 1:AA:314:C:C6      | 2.35                     | 0.62              |
| 1:AA:384:G:H2'     | 1:AA:385:C:C6      | 2.35                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:492:C:C2'    | 1:AA:493:A:H5''   | 2.28                     | 0.62              |
| 1:AA:590:U:H2'    | 1:AA:591:U:C6     | 2.35                     | 0.62              |
| 1:AA:1238:A:C2    | 1:AA:1241:G:H1'   | 2.35                     | 0.62              |
| 3:AD:2:ARG:HH12   | 3:AD:114:ARG:HD2  | 1.65                     | 0.62              |
| 6:AG:115:MET:HE3  | 6:AG:119:LEU:HB2  | 1.82                     | 0.62              |
| 9:AJ:88:MET:HB2   | 9:AJ:89:ARG:NH1   | 2.15                     | 0.62              |
| 10:AK:56:LYS:O    | 10:AK:58:THR:HG22 | 1.99                     | 0.62              |
| 14:AO:87:ARG:HA   | 14:AO:87:ARG:HH11 | 1.65                     | 0.62              |
| 15:AP:46:LYS:H    | 15:AP:46:LYS:CE   | 2.12                     | 0.62              |
| 15:AP:46:LYS:HE2  | 15:AP:46:LYS:N    | 2.15                     | 0.62              |
| 16:AQ:26:ARG:HH21 | 16:AQ:39:ARG:CZ   | 2.12                     | 0.62              |
| 21:AU:36:PHE:HB3  | 21:AU:40:PRO:CG   | 2.30                     | 0.62              |
| 23:BB:189:G:OP2   | 46:BZ:12:ILE:HG12 | 1.99                     | 0.62              |
| 23:BB:436:C:O2'   | 23:BB:437:U:H5'   | 2.00                     | 0.62              |
| 23:BB:438:G:H2'   | 23:BB:439:A:H8    | 1.65                     | 0.62              |
| 23:BB:1722:A:N6   | 23:BB:1738:G:H1'  | 2.15                     | 0.62              |
| 23:BB:2472:G:H2'  | 23:BB:2475:C:H42  | 1.64                     | 0.62              |
| 25:BC:43:ASN:OD1  | 25:BC:51:ARG:HD3  | 1.99                     | 0.62              |
| 25:BC:179:GLU:CG  | 25:BC:266:ILE:HA  | 2.30                     | 0.62              |
| 25:BC:179:GLU:HG3 | 25:BC:266:ILE:HA  | 1.82                     | 0.62              |
| 26:BD:48:ILE:HG13 | 26:BD:80:TRP:NE1  | 2.15                     | 0.62              |
| 29:BG:124:CYS:HB3 | 29:BG:129:GLU:O   | 1.99                     | 0.62              |
| 34:BM:69:PRO:HB2  | 34:BM:71:LYS:HZ1  | 1.65                     | 0.62              |
| 40:BS:88:ARG:HD2  | 40:BS:93:ALA:HB3  | 1.81                     | 0.62              |
| 43:BW:76:ARG:HG2  | 43:BW:77:LYS:N    | 2.13                     | 0.62              |
| 45:BY:9:THR:CA    | 45:BY:55:LYS:HE2  | 2.29                     | 0.62              |
| 1:CA:168:G:O2'    | 1:CA:169:C:H5'    | 1.99                     | 0.62              |
| 1:CA:1200:C:C4'   | 1:CA:1201:A:H5'   | 2.29                     | 0.62              |
| 2:CC:150:VAL:HG22 | 2:CC:199:VAL:HG12 | 1.82                     | 0.62              |
| 6:CG:11:ILE:HG21  | 6:CG:27:ASN:HD21  | 1.65                     | 0.62              |
| 6:CG:87:PRO:HG3   | 6:CG:148:LYS:HA   | 1.81                     | 0.62              |
| 19:CT:3:ILE:O     | 19:CT:4:LYS:HB2   | 2.00                     | 0.62              |
| 23:DB:3:U:H2'     | 23:DB:4:U:C6      | 2.34                     | 0.62              |
| 23:DB:401:A:H2'   | 23:DB:402:A:H8    | 1.65                     | 0.62              |
| 23:DB:664:G:H2'   | 23:DB:665:U:H6    | 1.65                     | 0.62              |
| 23:DB:1181:U:H2'  | 23:DB:1182:G:C8   | 2.35                     | 0.62              |
| 23:DB:1819:A:OP1  | 25:DC:153:LEU:HB2 | 1.99                     | 0.62              |
| 23:DB:2425:A:H5'  | 23:DB:2427:C:O4'  | 2.00                     | 0.62              |
| 28:DF:65:LEU:HD23 | 28:DF:87:LYS:HD2  | 1.80                     | 0.62              |
| 29:DG:94:ARG:HB2  | 29:DG:105:SER:HB2 | 1.82                     | 0.62              |
| 30:DH:4:ILE:HD11  | 30:DH:37:VAL:HA   | 1.81                     | 0.62              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 34:DM:133:LYS:HD2  | 34:DM:134:THR:O   | 2.00                     | 0.62              |
| 42:DU:9:GLU:HB2    | 42:DU:71:ILE:HG13 | 1.82                     | 0.62              |
| 43:DW:55:ASP:CG    | 43:DW:56:HIS:H    | 2.08                     | 0.62              |
| 48:D1:15:GLY:HA3   | 48:D1:47:ILE:HG21 | 1.82                     | 0.62              |
| 49:D2:17:GLY:O     | 49:D2:19:ARG:N    | 2.32                     | 0.62              |
| 1:AA:275:G:O5'     | 16:AQ:15:LYS:HG2  | 2.00                     | 0.61              |
| 1:AA:1182:G:H4'    | 1:AA:1183:U:H5'   | 1.81                     | 0.61              |
| 11:AL:43:LYS:N     | 11:AL:44:PRO:HD2  | 2.15                     | 0.61              |
| 19:AT:70:LYS:HB2   | 19:AT:70:LYS:NZ   | 2.13                     | 0.61              |
| 23:BB:1117:C:H2'   | 23:BB:1118:C:H6   | 1.65                     | 0.61              |
| 23:BB:1295:C:H2'   | 23:BB:1296:G:H8   | 1.65                     | 0.61              |
| 23:BB:1551:A:C3'   | 23:BB:1552:A:H5'' | 2.30                     | 0.61              |
| 23:BB:2743:U:H2'   | 23:BB:2744:G:O4'  | 2.00                     | 0.61              |
| 25:BC:103:ILE:HG22 | 25:BC:104:LEU:N   | 2.15                     | 0.61              |
| 26:BD:23:PRO:HB3   | 26:BD:189:VAL:N   | 2.15                     | 0.61              |
| 33:BL:61:LEU:H     | 33:BL:61:LEU:HD22 | 1.64                     | 0.61              |
| 42:BU:5:ARG:CG     | 42:BU:6:ARG:H     | 2.13                     | 0.61              |
| 43:BW:16:GLU:CG    | 43:BW:37:VAL:HG22 | 2.30                     | 0.61              |
| 47:B0:41:HIS:HD2   | 47:B0:42:ILE:HG22 | 1.65                     | 0.61              |
| 52:BI:116:MET:HE1  | 52:BI:124:MET:O   | 1.99                     | 0.61              |
| 1:CA:33:A:H1'      | 11:CL:27:PRO:HG3  | 1.81                     | 0.61              |
| 1:CA:590:U:H2'     | 1:CA:591:U:C6     | 2.35                     | 0.61              |
| 2:CC:18:ASN:O      | 2:CC:55:VAL:HA    | 2.00                     | 0.61              |
| 6:CG:125:ASP:HB3   | 6:CG:129:ASN:HA   | 1.83                     | 0.61              |
| 7:CH:6:ILE:HD11    | 7:CH:31:LEU:HD23  | 1.82                     | 0.61              |
| 23:DB:30:G:H2'     | 23:DB:31:C:C6     | 2.34                     | 0.61              |
| 23:DB:925:A:O2'    | 23:DB:926:G:H5'   | 2.00                     | 0.61              |
| 23:DB:1164:C:H2'   | 23:DB:1165:A:C8   | 2.36                     | 0.61              |
| 23:DB:1254:A:N1    | 27:DE:77:ILE:HD12 | 2.14                     | 0.61              |
| 23:DB:1439:A:N7    | 23:DB:1440:U:C6   | 2.68                     | 0.61              |
| 23:DB:1779:U:H5    | 23:DB:1784:A:N7   | 1.97                     | 0.61              |
| 23:DB:2008:C:H2'   | 23:DB:2009:A:C8   | 2.31                     | 0.61              |
| 23:DB:2405:G:H5'   | 33:DL:70:LYS:HG3  | 1.81                     | 0.61              |
| 23:DB:2678:C:H2'   | 23:DB:2679:A:C8   | 2.35                     | 0.61              |
| 25:DC:210:ALA:HA   | 25:DC:213:ARG:HD2 | 1.82                     | 0.61              |
| 28:DF:177:ARG:NH2  | 28:DF:178:LYS:HA  | 2.14                     | 0.61              |
| 34:DM:96:ILE:HD12  | 34:DM:96:ILE:N    | 2.15                     | 0.61              |
| 36:DO:15:ARG:HH12  | 43:DW:76:ARG:HE   | 1.45                     | 0.61              |
| 38:DQ:36:GLN:O     | 38:DQ:39:ILE:HG23 | 1.99                     | 0.61              |
| 43:DW:36:ILE:HG13  | 43:DW:38:ARG:H    | 1.65                     | 0.61              |
| 48:D1:19:PHE:HD1   | 48:D1:20:TYR:H    | 1.48                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:16:A:O2'      | 4:AE:20:VAL:HG13   | 2.00                     | 0.61              |
| 1:AA:32:A:H2'      | 1:AA:33:A:C8       | 2.34                     | 0.61              |
| 2:AC:133:MET:HE2   | 2:AC:152:VAL:HG21  | 1.82                     | 0.61              |
| 7:AH:8:ASP:OD2     | 7:AH:12:ARG:HD2    | 1.99                     | 0.61              |
| 7:AH:111:THR:H     | 7:AH:114:ALA:HB3   | 1.64                     | 0.61              |
| 8:AI:80:HIS:O      | 8:AI:84:ARG:HB2    | 1.99                     | 0.61              |
| 16:AQ:10:ARG:HA    | 16:AQ:10:ARG:NE    | 2.15                     | 0.61              |
| 20:AB:87:ASP:O     | 20:AB:88:GLN:HG3   | 2.01                     | 0.61              |
| 23:BB:1439:A:N7    | 23:BB:1440:U:C6    | 2.68                     | 0.61              |
| 23:BB:1682:G:H2'   | 23:BB:1683:U:C6    | 2.35                     | 0.61              |
| 23:BB:1722:A:H2'   | 23:BB:1723:G:C8    | 2.34                     | 0.61              |
| 24:BV:17:SER:HB3   | 24:BV:21:ARG:HH12  | 1.65                     | 0.61              |
| 25:BC:70:LYS:HE3   | 25:BC:95:TYR:CE2   | 2.35                     | 0.61              |
| 26:BD:22:ILE:N     | 26:BD:23:PRO:CD    | 2.63                     | 0.61              |
| 26:BD:33:ARG:HG3   | 26:BD:34:VAL:H     | 1.64                     | 0.61              |
| 26:BD:60:VAL:HB    | 26:BD:63:PRO:HG2   | 1.80                     | 0.61              |
| 27:BE:52:VAL:C     | 27:BE:54:GLY:H     | 2.08                     | 0.61              |
| 27:BE:57:LYS:HA    | 27:BE:57:LYS:HE3   | 1.81                     | 0.61              |
| 27:BE:105:LEU:HD22 | 27:BE:177:PRO:HG2  | 1.81                     | 0.61              |
| 29:BG:18:ILE:HA    | 29:BG:23:ILE:HD13  | 1.82                     | 0.61              |
| 29:BG:86:LEU:HD12  | 29:BG:161:VAL:HG12 | 1.82                     | 0.61              |
| 41:BT:13:ALA:O     | 41:BT:32:LEU:HA    | 2.00                     | 0.61              |
| 52:BI:135:MET:HG3  | 52:BI:137:LEU:HG   | 1.82                     | 0.61              |
| 1:CA:60:A:H4'      | 1:CA:61:G:O5'      | 2.00                     | 0.61              |
| 1:CA:859:G:H2'     | 1:CA:860:A:H8      | 1.65                     | 0.61              |
| 1:CA:1437:A:H2'    | 1:CA:1438:G:H8     | 1.65                     | 0.61              |
| 7:CH:124:ILE:HD12  | 7:CH:125:ILE:N     | 2.15                     | 0.61              |
| 12:CM:6:ILE:O      | 12:CM:8:ILE:HG23   | 2.00                     | 0.61              |
| 15:CP:68:SER:OG    | 15:CP:71:VAL:HG12  | 2.00                     | 0.61              |
| 21:CU:17:ARG:H     | 21:CU:17:ARG:CD    | 2.09                     | 0.61              |
| 23:DB:222:A:H61    | 23:DB:232:G:H1'    | 1.62                     | 0.61              |
| 23:DB:448:U:H3'    | 27:DE:79:ARG:HE    | 1.63                     | 0.61              |
| 23:DB:620:G:H5'    | 23:DB:620:G:N3     | 2.15                     | 0.61              |
| 23:DB:1064:C:H4'   | 52:DI:90:GLY:CA    | 2.28                     | 0.61              |
| 23:DB:1225:G:OP1   | 39:DR:90:ARG:HD2   | 2.00                     | 0.61              |
| 23:DB:1797:G:O3'   | 25:DC:253:GLY:HA2  | 1.99                     | 0.61              |
| 23:DB:2324:U:H3'   | 23:DB:2325:G:H5''  | 1.82                     | 0.61              |
| 23:DB:2755:C:H2'   | 51:D4:19:ARG:HH21  | 1.64                     | 0.61              |
| 26:DD:27:ILE:HG12  | 26:DD:185:ASN:O    | 2.00                     | 0.61              |
| 27:DE:77:ILE:HG12  | 27:DE:77:ILE:O     | 1.99                     | 0.61              |
| 28:DF:67:THR:OG1   | 28:DF:85:GLY:HA3   | 1.99                     | 0.61              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 29:DG:175:LYS:HG2  | 29:DG:176:LYS:N   | 2.14                     | 0.61              |
| 31:DJ:45:THR:HG22  | 31:DJ:47:HIS:H    | 1.65                     | 0.61              |
| 31:DJ:96:ARG:HG3   | 31:DJ:98:GLU:OE1  | 1.99                     | 0.61              |
| 33:DL:78:ARG:NE    | 33:DL:113:ALA:HB1 | 2.14                     | 0.61              |
| 42:DU:9:GLU:HB2    | 42:DU:71:ILE:CB   | 2.30                     | 0.61              |
| 44:DX:44:LYS:HG2   | 44:DX:47:ARG:HB2  | 1.82                     | 0.61              |
| 52:DI:121:ILE:HD13 | 52:DI:121:ILE:N   | 2.15                     | 0.61              |
| 1:AA:1506:U:H4'    | 10:AK:128:VAL:OXT | 2.00                     | 0.61              |
| 3:AD:99:ASN:CG     | 3:AD:103:ARG:HH21 | 2.07                     | 0.61              |
| 5:AF:4:TYR:O       | 5:AF:63:ASN:HA    | 2.00                     | 0.61              |
| 9:AJ:31:ARG:HH11   | 9:AJ:31:ARG:HG2   | 1.65                     | 0.61              |
| 9:AJ:53:ILE:HG12   | 9:AJ:63:ASP:HB2   | 1.82                     | 0.61              |
| 10:AK:36:ARG:HG2   | 10:AK:37:GLN:H    | 1.65                     | 0.61              |
| 10:AK:69:CYS:C     | 10:AK:71:ASP:H    | 2.06                     | 0.61              |
| 14:AO:55:LEU:O     | 14:AO:59:VAL:HG23 | 2.00                     | 0.61              |
| 23:BB:198:C:O2'    | 23:BB:199:A:H5''  | 2.00                     | 0.61              |
| 23:BB:526:A:N6     | 23:BB:2626:C:H4'  | 2.16                     | 0.61              |
| 23:BB:972:A:C3'    | 23:BB:973:A:H5''  | 2.30                     | 0.61              |
| 23:BB:1405:U:H2'   | 23:BB:1406:U:C6   | 2.36                     | 0.61              |
| 23:BB:1791:A:C2    | 23:BB:1829:A:H4'  | 2.35                     | 0.61              |
| 23:BB:1915:U:H3'   | 23:BB:1916:A:H8   | 1.66                     | 0.61              |
| 23:BB:2455:G:H2'   | 23:BB:2456:C:C6   | 2.36                     | 0.61              |
| 25:BC:37:SER:OG    | 25:BC:62:ARG:HG3  | 2.00                     | 0.61              |
| 26:BD:128:ARG:NH2  | 26:BD:130:GLN:HG3 | 2.14                     | 0.61              |
| 27:BE:186:VAL:O    | 27:BE:188:MET:HE3 | 1.99                     | 0.61              |
| 36:BO:49:VAL:HG22  | 36:BO:50:ALA:N    | 2.13                     | 0.61              |
| 42:BU:40:LEU:O     | 42:BU:42:LYS:HD2  | 2.00                     | 0.61              |
| 47:B0:6:LYS:HA     | 47:B0:6:LYS:HZ3   | 1.65                     | 0.61              |
| 48:B1:13:SER:N     | 48:B1:50:GLU:HA   | 2.15                     | 0.61              |
| 1:CA:673:A:H4'     | 5:CF:86:ARG:HD2   | 1.81                     | 0.61              |
| 1:CA:841:C:H3'     | 1:CA:843:U:OP2    | 1.99                     | 0.61              |
| 1:CA:1030:U:H5''   | 1:CA:1031:C:C5    | 2.34                     | 0.61              |
| 1:CA:1078:U:H4'    | 4:CE:137:ARG:HH12 | 1.66                     | 0.61              |
| 1:CA:1151:A:O2'    | 1:CA:1152:A:H5''  | 2.00                     | 0.61              |
| 1:CA:1287:A:H2'    | 1:CA:1288:A:C8    | 2.35                     | 0.61              |
| 21:CU:24:LYS:CD    | 21:CU:25:ALA:H    | 2.11                     | 0.61              |
| 23:DB:144:A:C6     | 41:DT:3:ARG:NH1   | 2.68                     | 0.61              |
| 23:DB:453:A:H4'    | 23:DB:472:A:N6    | 2.15                     | 0.61              |
| 23:DB:784:G:O2'    | 23:DB:785:G:H5''  | 2.01                     | 0.61              |
| 23:DB:912:C:O2'    | 23:DB:913:U:H5'   | 1.99                     | 0.61              |
| 23:DB:1099:G:H8    | 52:DI:3:LYS:CB    | 2.13                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DB:1116:G:H21   | 34:DM:136:MET:HE3 | 1.65                     | 0.61              |
| 23:DB:1722:A:N6    | 23:DB:1738:G:H1'  | 2.15                     | 0.61              |
| 23:DB:2293:G:H5''  | 36:DO:9:ARG:HH21  | 1.64                     | 0.61              |
| 31:DJ:117:ALA:C    | 31:DJ:121:LYS:HZ3 | 2.09                     | 0.61              |
| 33:DL:18:ARG:HH22  | 33:DL:21:ARG:HD3  | 1.65                     | 0.61              |
| 33:DL:62:PRO:HB3   | 50:D3:12:ARG:NE   | 2.16                     | 0.61              |
| 43:DW:67:LYS:HD2   | 43:DW:70:VAL:N    | 2.15                     | 0.61              |
| 1:AA:642:A:H2'     | 1:AA:643:C:C6     | 2.35                     | 0.61              |
| 1:AA:1074:G:H2'    | 1:AA:1075:U:C6    | 2.35                     | 0.61              |
| 20:AB:202:ASN:HD22 | 20:AB:202:ASN:C   | 2.08                     | 0.61              |
| 23:BB:18:U:H2'     | 23:BB:19:A:H8     | 1.64                     | 0.61              |
| 23:BB:1105:U:H2'   | 23:BB:1106:G:C8   | 2.34                     | 0.61              |
| 23:BB:1791:A:OP1   | 25:BC:211:ARG:HG2 | 2.00                     | 0.61              |
| 23:BB:2809:A:H2'   | 23:BB:2810:A:C8   | 2.36                     | 0.61              |
| 26:BD:128:ARG:HE   | 26:BD:128:ARG:CA  | 2.13                     | 0.61              |
| 26:BD:170:VAL:HG11 | 26:BD:194:PRO:CB  | 2.29                     | 0.61              |
| 34:BM:42:THR:CG2   | 34:BM:45:GLN:HB2  | 2.30                     | 0.61              |
| 39:BR:53:PHE:CE2   | 39:BR:54:VAL:HB   | 2.36                     | 0.61              |
| 43:BW:54:ARG:HH11  | 43:BW:54:ARG:HG2  | 1.65                     | 0.61              |
| 43:BW:66:VAL:HG22  | 43:BW:67:LYS:H    | 1.64                     | 0.61              |
| 50:B3:2:LYS:O      | 50:B3:2:LYS:HD3   | 2.00                     | 0.61              |
| 1:CA:105:G:H2'     | 1:CA:106:C:H6     | 1.64                     | 0.61              |
| 20:CB:10:LYS:HB2   | 20:CB:211:LEU:CD2 | 2.30                     | 0.61              |
| 20:CB:23:ASN:HD22  | 20:CB:24:PRO:HD2  | 1.63                     | 0.61              |
| 22:DA:65:U:O2'     | 22:DA:66:A:H5'    | 1.99                     | 0.61              |
| 23:DB:358:U:H2'    | 23:DB:359:G:C8    | 2.35                     | 0.61              |
| 23:DB:876:C:C2     | 23:DB:877:A:H1'   | 2.35                     | 0.61              |
| 23:DB:937:C:H2'    | 23:DB:938:G:H8    | 1.65                     | 0.61              |
| 23:DB:1201:U:H2'   | 23:DB:1202:G:C8   | 2.35                     | 0.61              |
| 24:DV:53:LYS:HZ2   | 24:DV:53:LYS:HB3  | 1.66                     | 0.61              |
| 25:DC:136:VAL:C    | 25:DC:138:SER:H   | 2.09                     | 0.61              |
| 25:DC:136:VAL:HA   | 25:DC:165:ALA:HA  | 1.82                     | 0.61              |
| 30:DH:3:VAL:HB     | 30:DH:37:VAL:CG1  | 2.31                     | 0.61              |
| 30:DH:51:ARG:HH11  | 30:DH:51:ARG:HG2  | 1.65                     | 0.61              |
| 30:DH:131:SER:HB2  | 30:DH:141:LYS:HA  | 1.81                     | 0.61              |
| 33:DL:33:ARG:HG2   | 39:DR:85:LYS:HZ3  | 1.64                     | 0.61              |
| 34:DM:28:PHE:HB2   | 34:DM:102:LEU:HG  | 1.82                     | 0.61              |
| 38:DQ:25:GLY:HA2   | 38:DQ:29:ARG:HD2  | 1.82                     | 0.61              |
| 39:DR:65:ALA:CB    | 39:DR:99:THR:HG23 | 2.25                     | 0.61              |
| 39:DR:71:LYS:HB2   | 39:DR:73:LYS:HZ1  | 1.64                     | 0.61              |
| 40:DS:21:ALA:HB1   | 40:DS:74:ILE:HD12 | 1.82                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:1040:U:H2'    | 1:AA:1041:G:H8    | 1.66                     | 0.61              |
| 8:AI:4:GLN:HG2     | 8:AI:21:LYS:HG3   | 1.81                     | 0.61              |
| 10:AK:18:GLY:O     | 10:AK:81:LEU:HB2  | 2.00                     | 0.61              |
| 22:BA:27:C:H5'     | 36:BO:34:HIS:CE1  | 2.35                     | 0.61              |
| 22:BA:104:A:H2'    | 22:BA:105:G:O4'   | 2.00                     | 0.61              |
| 23:BB:37:C:O2'     | 27:BE:46:GLN:HB3  | 2.00                     | 0.61              |
| 23:BB:831:G:O3'    | 33:BL:44:GLY:HA3  | 2.00                     | 0.61              |
| 23:BB:1439:A:C4    | 23:BB:1552:A:N6   | 2.69                     | 0.61              |
| 23:BB:1656:C:H5''  | 26:BD:141:ARG:HB3 | 1.83                     | 0.61              |
| 23:BB:1712:U:H3'   | 23:BB:1713:A:H5'' | 1.83                     | 0.61              |
| 23:BB:1838:C:N4    | 23:BB:1898:U:H2'  | 2.15                     | 0.61              |
| 23:BB:2365:G:H4'   | 43:BW:65:LYS:HZ2  | 1.65                     | 0.61              |
| 25:BC:15:VAL:HG12  | 25:BC:16:VAL:HG23 | 1.80                     | 0.61              |
| 25:BC:220:ARG:HA   | 25:BC:220:ARG:NE  | 2.15                     | 0.61              |
| 26:BD:128:ARG:HH22 | 26:BD:130:GLN:CG  | 2.13                     | 0.61              |
| 27:BE:130:LYS:HD3  | 27:BE:132:LYS:HD2 | 1.82                     | 0.61              |
| 28:BF:108:PRO:HB3  | 28:BF:113:PHE:CE2 | 2.36                     | 0.61              |
| 30:BH:132:PHE:HB3  | 30:BH:140:ALA:HB3 | 1.82                     | 0.61              |
| 45:BY:16:LEU:HD12  | 45:BY:16:LEU:N    | 2.16                     | 0.61              |
| 1:CA:974:A:C4'     | 1:CA:975:A:H5'    | 2.18                     | 0.61              |
| 1:CA:1154:G:O2'    | 1:CA:1155:A:H5'   | 2.01                     | 0.61              |
| 3:CD:130:ASN:H     | 3:CD:130:ASN:HD22 | 1.49                     | 0.61              |
| 11:CL:64:SER:OG    | 11:CL:96:THR:HG23 | 2.01                     | 0.61              |
| 23:DB:136:G:H21    | 41:DT:3:ARG:HG2   | 1.66                     | 0.61              |
| 23:DB:361:G:H2'    | 23:DB:362:A:H8    | 1.64                     | 0.61              |
| 23:DB:1405:U:H2'   | 23:DB:1406:U:C6   | 2.36                     | 0.61              |
| 23:DB:1656:C:OP1   | 26:DD:141:ARG:HD2 | 2.00                     | 0.61              |
| 23:DB:2574:G:N2    | 26:DD:147:GLY:HA3 | 2.11                     | 0.61              |
| 23:DB:2678:C:H2'   | 23:DB:2679:A:H8   | 1.64                     | 0.61              |
| 24:DV:48:MET:SD    | 24:DV:86:LEU:HD12 | 2.40                     | 0.61              |
| 29:DG:30:GLY:H     | 29:DG:78:VAL:HG23 | 1.65                     | 0.61              |
| 30:DH:11:ASN:HD22  | 30:DH:20:ASN:ND2  | 1.97                     | 0.61              |
| 30:DH:37:VAL:O     | 30:DH:38:PRO:C    | 2.43                     | 0.61              |
| 45:DY:15:ARG:NE    | 45:DY:15:ARG:HA   | 2.16                     | 0.61              |
| 48:D1:24:LYS:HZ2   | 48:D1:24:LYS:C    | 2.08                     | 0.61              |
| 1:AA:22:G:H4'      | 1:AA:885:G:C8     | 2.36                     | 0.61              |
| 1:AA:1011:C:H2'    | 1:AA:1012:A:H8    | 1.65                     | 0.61              |
| 1:AA:1132:C:H2'    | 1:AA:1133:G:O4'   | 2.00                     | 0.61              |
| 1:AA:1182:G:H4'    | 1:AA:1183:U:C5'   | 2.30                     | 0.61              |
| 1:AA:1217:C:OP1    | 13:AN:8:ARG:HD3   | 2.01                     | 0.61              |
| 1:AA:1320:C:C5     | 18:AS:36:ARG:HG2  | 2.36                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:AF:6:ILE:HD13    | 5:AF:89:VAL:HB     | 1.83                     | 0.61              |
| 23:BB:1105:U:H2'   | 23:BB:1106:G:H8    | 1.65                     | 0.61              |
| 23:BB:2425:A:H5'   | 23:BB:2427:C:O4'   | 2.00                     | 0.61              |
| 26:BD:23:PRO:HG2   | 26:BD:178:VAL:HG21 | 1.81                     | 0.61              |
| 26:BD:48:ILE:HG13  | 26:BD:80:TRP:HE1   | 1.64                     | 0.61              |
| 26:BD:129:THR:O    | 26:BD:140:HIS:HA   | 2.01                     | 0.61              |
| 27:BE:147:LEU:HD13 | 27:BE:183:PHE:HA   | 1.83                     | 0.61              |
| 28:BF:126:ASN:H    | 28:BF:126:ASN:ND2  | 1.98                     | 0.61              |
| 33:BL:126:ARG:NH2  | 33:BL:131:ALA:HB2  | 2.16                     | 0.61              |
| 37:BP:38:ARG:HG3   | 37:BP:39:LEU:N     | 2.15                     | 0.61              |
| 38:BQ:39:ILE:HG23  | 39:BR:80:ARG:HD3   | 1.82                     | 0.61              |
| 39:BR:84:ARG:NH1   | 39:BR:86:GLN:HB3   | 2.15                     | 0.61              |
| 40:BS:6:LYS:HB3    | 40:BS:6:LYS:HZ2    | 1.66                     | 0.61              |
| 1:CA:1023:U:H2'    | 1:CA:1024:G:C8     | 2.35                     | 0.61              |
| 12:CM:9:PRO:HB2    | 12:CM:17:ALA:HB1   | 1.83                     | 0.61              |
| 23:DB:64:A:C5'     | 41:DT:76:ARG:HD2   | 2.30                     | 0.61              |
| 23:DB:104:A:H2'    | 23:DB:105:C:H6     | 1.66                     | 0.61              |
| 23:DB:544:C:H4'    | 23:DB:545:U:OP1    | 2.00                     | 0.61              |
| 23:DB:2393:U:H4'   | 33:DL:62:PRO:O     | 2.01                     | 0.61              |
| 33:DL:34:GLY:HA3   | 39:DR:85:LYS:HE2   | 1.82                     | 0.61              |
| 33:DL:110:VAL:HG22 | 33:DL:127:VAL:HA   | 1.82                     | 0.61              |
| 42:DU:4:ILE:HG22   | 42:DU:27:VAL:HG22  | 1.81                     | 0.61              |
| 1:AA:1506:U:H4'    | 10:AK:128:VAL:C    | 2.26                     | 0.61              |
| 7:AH:82:LEU:HD13   | 7:AH:82:LEU:O      | 1.99                     | 0.61              |
| 10:AK:111:ASP:HB2  | 21:AU:16:ARG:NH2   | 2.15                     | 0.61              |
| 19:AT:81:GLN:O     | 19:AT:85:LEU:HB3   | 2.01                     | 0.61              |
| 23:BB:322:A:H5'    | 23:BB:340:A:H1'    | 1.83                     | 0.61              |
| 23:BB:527:C:H5''   | 23:BB:2779:U:O2    | 2.00                     | 0.61              |
| 23:BB:664:G:H2'    | 23:BB:665:U:H6     | 1.65                     | 0.61              |
| 23:BB:682:G:H5'    | 49:B2:26:ASN:CG    | 2.25                     | 0.61              |
| 23:BB:1015:U:H2'   | 23:BB:1016:G:C8    | 2.36                     | 0.61              |
| 24:BV:21:ARG:HA    | 24:BV:25:LYS:O     | 2.00                     | 0.61              |
| 26:BD:175:LEU:HD22 | 26:BD:189:VAL:HG12 | 1.81                     | 0.61              |
| 26:BD:187:LEU:HD23 | 26:BD:188:LEU:N    | 2.16                     | 0.61              |
| 31:BJ:73:VAL:HB    | 31:BJ:75:TYR:CE1   | 2.35                     | 0.61              |
| 32:BK:71:ARG:O     | 32:BK:72:PRO:C     | 2.44                     | 0.61              |
| 41:BT:65:GLY:O     | 41:BT:66:LYS:HB3   | 2.01                     | 0.61              |
| 43:BW:49:ASN:HB2   | 43:BW:53:GLY:HA3   | 1.82                     | 0.61              |
| 1:CA:1014:A:H4'    | 18:CS:13:HIS:CD2   | 2.36                     | 0.61              |
| 1:CA:1292:G:H2'    | 1:CA:1293:C:C6     | 2.35                     | 0.61              |
| 22:DA:25:U:H4'     | 22:DA:27:C:OP1     | 2.00                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DB:381:G:O2'   | 23:DB:382:A:H5'   | 2.00                     | 0.61              |
| 23:DB:918:A:H2'   | 23:DB:919:U:C5'   | 2.27                     | 0.61              |
| 23:DB:2471:A:O2'  | 23:DB:2472:G:O5'  | 2.19                     | 0.61              |
| 25:DC:3:VAL:HG21  | 25:DC:9:SER:HB3   | 1.82                     | 0.61              |
| 25:DC:20:ASN:CB   | 25:DC:202:ARG:HD3 | 2.31                     | 0.61              |
| 26:DD:14:ILE:HD12 | 37:DP:78:PRO:CG   | 2.30                     | 0.61              |
| 28:DF:140:ILE:H   | 28:DF:140:ILE:CD1 | 2.13                     | 0.61              |
| 31:DJ:73:VAL:HG22 | 31:DJ:74:TYR:N    | 2.16                     | 0.61              |
| 31:DJ:88:THR:HG23 | 31:DJ:92:MET:HE3  | 1.82                     | 0.61              |
| 33:DL:77:ILE:HD11 | 33:DL:109:LYS:HB2 | 1.83                     | 0.61              |
| 38:DQ:10:ARG:O    | 38:DQ:14:LYS:HB2  | 2.01                     | 0.61              |
| 39:DR:69:GLY:HA2  | 39:DR:97:LYS:H    | 1.66                     | 0.61              |
| 40:DS:36:LEU:HA   | 40:DS:39:THR:HG22 | 1.81                     | 0.61              |
| 45:DY:29:ARG:O    | 45:DY:33:HIS:HB3  | 2.00                     | 0.61              |
| 52:DI:27:LEU:HB2  | 52:DI:32:VAL:HG21 | 1.82                     | 0.61              |
| 1:AA:132:C:H5''   | 19:AT:68:LYS:HE3  | 1.83                     | 0.61              |
| 6:AG:114:SER:C    | 6:AG:118:ARG:HG3  | 2.26                     | 0.61              |
| 11:AL:3:VAL:O     | 11:AL:7:VAL:HG23  | 1.99                     | 0.61              |
| 12:AM:22:TYR:HB3  | 12:AM:69:ARG:NH2  | 2.15                     | 0.61              |
| 21:AU:38:GLU:C    | 21:AU:40:PRO:HD2  | 2.26                     | 0.61              |
| 23:BB:355:U:H2'   | 23:BB:356:G:C8    | 2.35                     | 0.61              |
| 23:BB:990:A:H1'   | 23:BB:1156:A:H2   | 1.65                     | 0.61              |
| 23:BB:1874:C:H2'  | 23:BB:1875:G:O4'  | 2.01                     | 0.61              |
| 23:BB:2291:U:H2'  | 23:BB:2292:U:C6   | 2.35                     | 0.61              |
| 23:BB:2423:U:H3   | 43:BW:1:ALA:HB2   | 1.66                     | 0.61              |
| 23:BB:2888:C:H2'  | 23:BB:2889:C:C6   | 2.36                     | 0.61              |
| 25:BC:23:LEU:HD12 | 25:BC:23:LEU:O    | 2.01                     | 0.61              |
| 26:BD:11:MET:HE2  | 26:BD:12:THR:O    | 2.01                     | 0.61              |
| 29:BG:5:LYS:HG2   | 29:BG:65:GLY:HA2  | 1.83                     | 0.61              |
| 33:BL:38:GLN:NE2  | 33:BL:39:LYS:H    | 1.98                     | 0.61              |
| 43:BW:23:LYS:NZ   | 43:BW:24:ARG:HG2  | 2.16                     | 0.61              |
| 52:BI:27:LEU:H    | 52:BI:27:LEU:CD2  | 2.11                     | 0.61              |
| 1:CA:313:A:H2'    | 1:CA:314:C:C6     | 2.35                     | 0.61              |
| 1:CA:1031:C:H4'   | 1:CA:1032:G:C5'   | 2.30                     | 0.61              |
| 1:CA:1342:C:H2'   | 1:CA:1343:G:C8    | 2.35                     | 0.61              |
| 17:CR:20:ILE:O    | 17:CR:21:ASP:HB2  | 2.00                     | 0.61              |
| 23:DB:285:G:H2'   | 23:DB:286:U:O4'   | 2.01                     | 0.61              |
| 23:DB:765:C:H2'   | 23:DB:766:U:H6    | 1.66                     | 0.61              |
| 23:DB:1229:C:H2'  | 23:DB:1230:A:C8   | 2.36                     | 0.61              |
| 23:DB:1821:A:H2'  | 23:DB:1822:C:C6   | 2.36                     | 0.61              |
| 23:DB:1838:C:N4   | 23:DB:1898:U:H2'  | 2.15                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:2472:G:H2'   | 23:DB:2475:C:H42   | 1.65                     | 0.61              |
| 25:DC:74:PRO:HG3   | 25:DC:116:GLN:HE21 | 1.64                     | 0.61              |
| 25:DC:257:ARG:HA   | 25:DC:261:ARG:CD   | 2.30                     | 0.61              |
| 26:DD:48:ILE:HA    | 26:DD:79:LEU:O     | 2.01                     | 0.61              |
| 29:DG:51:PHE:HE1   | 29:DG:53:PRO:HG3   | 1.66                     | 0.61              |
| 30:DH:66:ASN:HA    | 30:DH:138:VAL:HG22 | 1.83                     | 0.61              |
| 30:DH:122:LEU:HA   | 30:DH:146:VAL:HG21 | 1.83                     | 0.61              |
| 31:DJ:99:ARG:O     | 31:DJ:103:ILE:HG12 | 2.00                     | 0.61              |
| 33:DL:110:VAL:O    | 33:DL:111:ILE:HG12 | 2.00                     | 0.61              |
| 37:DP:5:LYS:HZ3    | 37:DP:5:LYS:HA     | 1.65                     | 0.61              |
| 45:DY:2:LYS:HD2    | 45:DY:35:VAL:HB    | 1.82                     | 0.61              |
| 46:DZ:62:LYS:HA    | 46:DZ:65:ASN:HD21  | 1.66                     | 0.61              |
| 1:AA:72:A:H2'      | 1:AA:73:C:C6       | 2.36                     | 0.61              |
| 10:AK:97:ARG:HB3   | 10:AK:97:ARG:HH11  | 1.66                     | 0.61              |
| 14:AO:2:LEU:HD23   | 14:AO:3:SER:N      | 2.16                     | 0.61              |
| 23:BB:557:C:O2'    | 31:BJ:114:LEU:HD13 | 2.01                     | 0.61              |
| 23:BB:620:G:N3     | 23:BB:620:G:H5'    | 2.15                     | 0.61              |
| 23:BB:670:A:H3'    | 33:BL:47:ARG:NH1   | 2.10                     | 0.61              |
| 23:BB:1019:U:H2'   | 23:BB:1020:A:C8    | 2.36                     | 0.61              |
| 23:BB:2308:G:H5'   | 23:BB:2309:A:H5''  | 1.82                     | 0.61              |
| 23:BB:2471:A:O2'   | 23:BB:2472:G:O5'   | 2.19                     | 0.61              |
| 23:BB:2839:G:H21   | 35:BN:92:GLY:HA3   | 1.64                     | 0.61              |
| 25:BC:194:VAL:HG12 | 25:BC:195:GLY:N    | 2.16                     | 0.61              |
| 26:BD:132:ALA:HA   | 26:BD:136:ASN:H    | 1.65                     | 0.61              |
| 33:BL:91:ASP:OD2   | 33:BL:123:ARG:HD2  | 2.01                     | 0.61              |
| 33:BL:103:ILE:O    | 33:BL:104:GLN:HB3  | 2.00                     | 0.61              |
| 34:BM:34:LYS:HA    | 34:BM:99:GLY:HA3   | 1.83                     | 0.61              |
| 35:BN:98:LEU:O     | 35:BN:111:ALA:HA   | 2.01                     | 0.61              |
| 44:BX:45:GLN:H     | 44:BX:45:GLN:HE21  | 1.49                     | 0.61              |
| 50:B3:34:LYS:C     | 50:B3:35:LYS:HD3   | 2.25                     | 0.61              |
| 1:CA:900:A:O2'     | 1:CA:901:A:H5'     | 2.00                     | 0.61              |
| 9:CJ:64:GLN:HB3    | 13:CN:98:ALA:HB3   | 1.83                     | 0.61              |
| 16:CQ:10:ARG:CZ    | 16:CQ:55:GLY:H     | 2.13                     | 0.61              |
| 20:CB:36:LYS:HE3   | 20:CB:36:LYS:N     | 2.16                     | 0.61              |
| 23:DB:291:G:O2'    | 23:DB:292:U:H5'    | 2.01                     | 0.61              |
| 23:DB:1019:U:H2'   | 23:DB:1020:A:C8    | 2.35                     | 0.61              |
| 23:DB:1439:A:C4    | 23:DB:1552:A:N6    | 2.69                     | 0.61              |
| 23:DB:2615:U:H1'   | 47:D0:3:GLN:HB3    | 1.83                     | 0.61              |
| 37:DP:23:ASP:HA    | 37:DP:49:ILE:CG2   | 2.30                     | 0.61              |
| 37:DP:112:ARG:HE   | 37:DP:112:ARG:N    | 1.98                     | 0.61              |
| 39:DR:6:GLN:N      | 39:DR:6:GLN:HE21   | 1.98                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:636:U:H2'     | 1:AA:637:C:H6      | 1.66                     | 0.61              |
| 1:AA:1137:C:O2'    | 1:AA:1138:G:H5''   | 2.00                     | 0.61              |
| 1:AA:1280:A:O4'    | 9:AJ:43:PRO:HG3    | 2.01                     | 0.61              |
| 8:AI:51:LEU:HD11   | 8:AI:82:ILE:HD13   | 1.83                     | 0.61              |
| 8:AI:99:LYS:HD3    | 8:AI:99:LYS:C      | 2.26                     | 0.61              |
| 23:BB:138:U:H2'    | 23:BB:140:C:H1'    | 1.83                     | 0.61              |
| 23:BB:143:C:H2'    | 23:BB:144:A:C8     | 2.36                     | 0.61              |
| 23:BB:224:U:O4     | 23:BB:420:C:H5'    | 2.00                     | 0.61              |
| 23:BB:743:A:O3'    | 26:BD:136:ASN:HB2  | 2.00                     | 0.61              |
| 23:BB:852:U:H2'    | 23:BB:853:C:C6     | 2.36                     | 0.61              |
| 23:BB:969:G:H2'    | 23:BB:970:U:H6     | 1.64                     | 0.61              |
| 23:BB:1038:G:H2'   | 23:BB:1039:A:C8    | 2.36                     | 0.61              |
| 23:BB:2047:C:H2'   | 23:BB:2048:G:H8    | 1.66                     | 0.61              |
| 23:BB:2318:G:O2'   | 23:BB:2319:G:N2    | 2.34                     | 0.61              |
| 27:BE:59:PRO:HD2   | 27:BE:60:TRP:NE1   | 2.16                     | 0.61              |
| 28:BF:97:GLU:O     | 28:BF:100:GLU:HG3  | 2.00                     | 0.61              |
| 33:BL:94:THR:O     | 33:BL:100:ILE:HG13 | 2.00                     | 0.61              |
| 37:BP:52:ARG:HB3   | 37:BP:60:VAL:CG1   | 2.22                     | 0.61              |
| 41:BT:45:ALA:O     | 41:BT:48:GLN:HB3   | 2.00                     | 0.61              |
| 50:B3:41:ARG:HB3   | 50:B3:43:LEU:CD2   | 2.30                     | 0.61              |
| 1:CA:56:U:H2'      | 1:CA:57:G:C8       | 2.36                     | 0.61              |
| 1:CA:1319:A:OP1    | 18:CS:4:LEU:HD21   | 2.00                     | 0.61              |
| 3:CD:160:LEU:HD13  | 3:CD:161:ALA:N     | 2.16                     | 0.61              |
| 4:CE:111:ARG:HH11  | 4:CE:111:ARG:HG2   | 1.66                     | 0.61              |
| 23:DB:401:A:H2'    | 23:DB:402:A:C8     | 2.35                     | 0.61              |
| 23:DB:898:C:C2'    | 23:DB:899:A:H5''   | 2.31                     | 0.61              |
| 23:DB:1252:G:N3    | 38:DQ:32:ARG:HG3   | 2.16                     | 0.61              |
| 23:DB:1712:U:H3'   | 23:DB:1713:A:H5''  | 1.83                     | 0.61              |
| 23:DB:1791:A:N6    | 23:DB:1828:G:H1'   | 2.16                     | 0.61              |
| 23:DB:2455:G:H2'   | 23:DB:2456:C:C6    | 2.35                     | 0.61              |
| 23:DB:2785:C:H2'   | 23:DB:2786:U:H6    | 1.65                     | 0.61              |
| 25:DC:12:ARG:HH11  | 25:DC:18:VAL:HB    | 1.66                     | 0.61              |
| 26:DD:70:LYS:HZ2   | 26:DD:70:LYS:HB3   | 1.64                     | 0.61              |
| 26:DD:174:SER:C    | 26:DD:175:LEU:HD12 | 2.25                     | 0.61              |
| 27:DE:5:LEU:HA     | 27:DE:11:ALA:O     | 2.00                     | 0.61              |
| 28:DF:133:GLU:HG2  | 28:DF:149:ARG:O    | 2.01                     | 0.61              |
| 29:DG:36:LEU:CB    | 29:DG:40:VAL:HG21  | 2.30                     | 0.61              |
| 32:DK:69:VAL:HG11  | 32:DK:106:GLU:CD   | 2.26                     | 0.61              |
| 34:DM:19:GLY:C     | 34:DM:20:LEU:HD12  | 2.25                     | 0.61              |
| 38:DQ:108:LEU:HD12 | 38:DQ:111:LYS:HD2  | 1.83                     | 0.61              |
| 41:DT:45:ALA:HA    | 41:DT:48:GLN:HG2   | 1.83                     | 0.61              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:DZ:55:GLY:CA    | 46:DZ:59:ARG:HB2   | 2.26                     | 0.61              |
| 47:D0:36:LYS:CB    | 47:D0:41:HIS:HA    | 2.31                     | 0.61              |
| 1:AA:160:A:H2'     | 1:AA:161:A:O4'     | 2.00                     | 0.60              |
| 1:AA:815:A:H4'     | 1:AA:817:C:C4      | 2.36                     | 0.60              |
| 8:AI:87:MET:SD     | 8:AI:94:ARG:HG3    | 2.42                     | 0.60              |
| 20:AB:67:LEU:HD21  | 20:AB:157:PRO:HG3  | 1.83                     | 0.60              |
| 23:BB:64:A:O2'     | 41:BT:69:ARG:HB3   | 2.01                     | 0.60              |
| 23:BB:1076:C:H4'   | 52:BI:94:LYS:HE3   | 1.81                     | 0.60              |
| 23:BB:1495:A:H2'   | 23:BB:1496:A:C8    | 2.35                     | 0.60              |
| 23:BB:1821:A:H2'   | 23:BB:1822:C:C6    | 2.36                     | 0.60              |
| 23:BB:2183:A:H2'   | 23:BB:2184:A:C8    | 2.36                     | 0.60              |
| 23:BB:2895:G:H2'   | 23:BB:2896:C:H6    | 1.64                     | 0.60              |
| 26:BD:34:VAL:HG11  | 26:BD:71:ALA:HB2   | 1.83                     | 0.60              |
| 30:BH:140:ALA:C    | 30:BH:141:LYS:HD3  | 2.26                     | 0.60              |
| 31:BJ:100:VAL:HG22 | 31:BJ:101:ILE:N    | 2.15                     | 0.60              |
| 33:BL:62:PRO:O     | 50:B3:24:LYS:HD3   | 2.01                     | 0.60              |
| 36:BO:35:ILE:N     | 36:BO:35:ILE:HD13  | 2.16                     | 0.60              |
| 38:BQ:33:VAL:HG13  | 38:BQ:34:ALA:N     | 2.09                     | 0.60              |
| 39:BR:18:GLN:NE2   | 39:BR:99:THR:HB    | 2.15                     | 0.60              |
| 52:BI:100:ILE:O    | 52:BI:139:VAL:HA   | 2.01                     | 0.60              |
| 1:CA:278:G:N2      | 1:CA:279:A:H62     | 1.97                     | 0.60              |
| 20:CB:36:LYS:HE3   | 20:CB:36:LYS:H     | 1.66                     | 0.60              |
| 22:DA:2:G:H2'      | 22:DA:3:C:C6       | 2.36                     | 0.60              |
| 23:DB:2339:C:H2'   | 23:DB:2340:A:C8    | 2.36                     | 0.60              |
| 25:DC:174:ARG:HG3  | 25:DC:180:MET:HG3  | 1.83                     | 0.60              |
| 25:DC:235:GLU:HG3  | 25:DC:237:ARG:HD3  | 1.82                     | 0.60              |
| 26:DD:73:VAL:HB    | 26:DD:91:THR:HB    | 1.83                     | 0.60              |
| 29:DG:36:LEU:HD12  | 29:DG:36:LEU:H     | 1.66                     | 0.60              |
| 30:DH:1:MET:HG3    | 30:DH:21:VAL:CG2   | 2.31                     | 0.60              |
| 31:DJ:49:ASP:HA    | 31:DJ:114:LEU:HD11 | 1.82                     | 0.60              |
| 32:DK:70:ARG:HB3   | 32:DK:76:VAL:HA    | 1.82                     | 0.60              |
| 35:DN:78:LYS:HG2   | 35:DN:82:GLU:HG3   | 1.83                     | 0.60              |
| 42:DU:4:ILE:CG2    | 42:DU:27:VAL:HG22  | 2.31                     | 0.60              |
| 1:AA:1053:G:H4'    | 1:AA:1054:C:H5'    | 1.83                     | 0.60              |
| 1:AA:1142:G:H2'    | 1:AA:1143:G:O4'    | 2.01                     | 0.60              |
| 3:AD:19:PHE:HB2    | 3:AD:110:ARG:HH12  | 1.66                     | 0.60              |
| 3:AD:122:ILE:O     | 3:AD:128:VAL:HG23  | 2.01                     | 0.60              |
| 7:AH:64:TYR:HA     | 7:AH:70:VAL:HG23   | 1.82                     | 0.60              |
| 10:AK:88:PRO:HA    | 10:AK:92:ARG:HE    | 1.65                     | 0.60              |
| 23:BB:445:C:O2'    | 23:BB:446:G:H5'    | 2.01                     | 0.60              |
| 23:BB:1474:U:H2'   | 23:BB:1475:G:H5'   | 1.84                     | 0.60              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BB:2081:U:H5'' | 46:BZ:23:LYS:HD2  | 1.82                     | 0.60              |
| 23:BB:2196:C:O2'  | 23:BB:2197:U:H5'  | 2.01                     | 0.60              |
| 23:BB:2270:A:H4'  | 43:BW:18:LYS:HB3  | 1.82                     | 0.60              |
| 23:BB:2298:A:N6   | 23:BB:2319:G:H22  | 1.99                     | 0.60              |
| 23:BB:2760:C:O2'  | 23:BB:2761:A:H5'  | 2.01                     | 0.60              |
| 23:BB:2785:C:H2'  | 23:BB:2786:U:H6   | 1.65                     | 0.60              |
| 25:BC:92:LEU:O    | 25:BC:93:VAL:HB   | 2.02                     | 0.60              |
| 31:BJ:84:ILE:HG22 | 31:BJ:85:LYS:N    | 2.16                     | 0.60              |
| 33:BL:56:PRO:HA   | 33:BL:60:ARG:NH2  | 2.16                     | 0.60              |
| 34:BM:109:PRO:HA  | 34:BM:112:LEU:HB2 | 1.83                     | 0.60              |
| 35:BN:9:GLN:NE2   | 35:BN:17:ARG:HH22 | 1.99                     | 0.60              |
| 35:BN:36:THR:O    | 35:BN:40:LYS:HB2  | 2.01                     | 0.60              |
| 36:BO:87:ILE:CG1  | 36:BO:88:LYS:H    | 2.14                     | 0.60              |
| 38:BQ:50:ARG:HA   | 38:BQ:53:LYS:HE3  | 1.83                     | 0.60              |
| 1:CA:57:G:H2'     | 1:CA:58:C:C6      | 2.35                     | 0.60              |
| 1:CA:77:A:H2'     | 1:CA:78:A:H8      | 1.66                     | 0.60              |
| 1:CA:636:U:H2'    | 1:CA:637:C:H6     | 1.66                     | 0.60              |
| 1:CA:642:A:H2'    | 1:CA:643:C:C6     | 2.35                     | 0.60              |
| 1:CA:1324:A:H5'   | 1:CA:1362:A:O2'   | 2.01                     | 0.60              |
| 21:CU:40:PRO:O    | 21:CU:44:ARG:N    | 2.34                     | 0.60              |
| 23:DB:6:A:H2'     | 23:DB:7:G:H8      | 1.65                     | 0.60              |
| 23:DB:393:C:O2'   | 23:DB:394:C:H5'   | 2.01                     | 0.60              |
| 23:DB:633:A:H2'   | 23:DB:634:C:H5'   | 1.82                     | 0.60              |
| 23:DB:1025:G:H1'  | 23:DB:1135:C:C5'  | 2.26                     | 0.60              |
| 23:DB:2293:G:OP1  | 36:DO:13:ARG:NH2  | 2.34                     | 0.60              |
| 23:DB:2621:G:O2'  | 26:DD:164:GLN:HG3 | 2.00                     | 0.60              |
| 23:DB:2680:U:H5'  | 26:DD:194:PRO:HA  | 1.83                     | 0.60              |
| 25:DC:117:SER:HB3 | 25:DC:127:ASN:ND2 | 2.17                     | 0.60              |
| 27:DE:14:VAL:HG12 | 27:DE:15:SER:N    | 2.16                     | 0.60              |
| 27:DE:109:LEU:HG  | 27:DE:117:ARG:HD3 | 1.82                     | 0.60              |
| 30:DH:135:HIS:HB3 | 30:DH:138:VAL:HB  | 1.83                     | 0.60              |
| 31:DJ:41:LYS:HZ3  | 31:DJ:45:THR:HA   | 1.67                     | 0.60              |
| 33:DL:78:ARG:HB3  | 33:DL:78:ARG:CZ   | 2.31                     | 0.60              |
| 37:DP:5:LYS:HA    | 37:DP:5:LYS:NZ    | 2.16                     | 0.60              |
| 41:DT:68:LYS:HB2  | 41:DT:68:LYS:HZ3  | 1.64                     | 0.60              |
| 43:DW:39:GLN:HG2  | 43:DW:66:VAL:O    | 2.01                     | 0.60              |
| 2:AC:26:LYS:HD3   | 2:AC:26:LYS:C     | 2.25                     | 0.60              |
| 9:AJ:15:HIS:HA    | 9:AJ:18:ILE:HG22  | 1.82                     | 0.60              |
| 11:AL:66:ILE:HD13 | 11:AL:73:LEU:HD12 | 1.84                     | 0.60              |
| 19:AT:4:LYS:HD2   | 19:AT:5:SER:N     | 2.16                     | 0.60              |
| 23:BB:28:A:N6     | 23:BB:512:G:O2'   | 2.33                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:BB:765:C:H2'    | 23:BB:766:U:H6    | 1.66                     | 0.60              |
| 23:BB:903:C:H2'    | 23:BB:904:G:C8    | 2.37                     | 0.60              |
| 23:BB:1857:G:H1'   | 23:BB:1885:A:N6   | 2.16                     | 0.60              |
| 23:BB:1857:G:H2'   | 23:BB:1884:G:H22  | 1.66                     | 0.60              |
| 23:BB:2785:C:H2'   | 23:BB:2786:U:C6   | 2.36                     | 0.60              |
| 25:BC:21:PRO:C     | 25:BC:202:ARG:HD2 | 2.25                     | 0.60              |
| 26:BD:3:GLY:HA2    | 26:BD:49:GLN:OE1  | 2.01                     | 0.60              |
| 36:BO:68:LYS:HD3   | 36:BO:68:LYS:N    | 2.16                     | 0.60              |
| 39:BR:64:VAL:HB    | 39:BR:98:ILE:HD12 | 1.84                     | 0.60              |
| 43:BW:45:HIS:HA    | 43:BW:75:ASN:CB   | 2.32                     | 0.60              |
| 48:B1:8:ILE:HD11   | 48:B1:25:ASN:HB3  | 1.82                     | 0.60              |
| 52:BI:10:LEU:HD13  | 52:BI:12:VAL:HG13 | 1.82                     | 0.60              |
| 1:CA:26:A:H61      | 1:CA:558:G:H1'    | 1.65                     | 0.60              |
| 1:CA:1176:A:H2'    | 1:CA:1177:G:O4'   | 2.01                     | 0.60              |
| 4:CE:12:GLU:HG2    | 4:CE:38:VAL:HG22  | 1.83                     | 0.60              |
| 7:CH:81:GLY:O      | 7:CH:82:LEU:HB2   | 2.02                     | 0.60              |
| 11:CL:80:LEU:O     | 11:CL:97:VAL:HG22 | 2.00                     | 0.60              |
| 23:DB:144:A:C2     | 41:DT:3:ARG:CZ    | 2.85                     | 0.60              |
| 23:DB:374:A:N6     | 23:DB:400:G:H1'   | 2.16                     | 0.60              |
| 23:DB:533:G:H5'    | 38:DQ:23:TYR:CD1  | 2.37                     | 0.60              |
| 23:DB:2354:C:H4'   | 43:DW:30:VAL:HG13 | 1.82                     | 0.60              |
| 23:DB:2650:U:H2'   | 23:DB:2651:C:C6   | 2.36                     | 0.60              |
| 23:DB:2789:C:H3'   | 23:DB:2893:A:H62  | 1.66                     | 0.60              |
| 23:DB:2809:A:H2'   | 23:DB:2810:A:C8   | 2.35                     | 0.60              |
| 25:DC:65:ASP:OD2   | 25:DC:101:ARG:HD3 | 2.01                     | 0.60              |
| 27:DE:143:LEU:HD22 | 27:DE:143:LEU:H   | 1.66                     | 0.60              |
| 28:DF:33:ILE:HD11  | 28:DF:99:PHE:HB2  | 1.83                     | 0.60              |
| 32:DK:102:PRO:CB   | 32:DK:121:GLU:HG2 | 2.30                     | 0.60              |
| 33:DL:96:LYS:HA    | 33:DL:96:LYS:HE3  | 1.81                     | 0.60              |
| 35:DN:2:ARG:HG2    | 35:DN:2:ARG:NH1   | 2.15                     | 0.60              |
| 39:DR:79:ARG:NH2   | 39:DR:87:GLN:HG3  | 2.15                     | 0.60              |
| 46:DZ:64:PHE:O     | 46:DZ:67:PRO:HD2  | 2.01                     | 0.60              |
| 50:D3:4:LYS:HZ2    | 50:D3:60:CYS:H    | 1.47                     | 0.60              |
| 1:AA:620:C:C6      | 3:AD:131:ILE:HD13 | 2.37                     | 0.60              |
| 1:AA:1526:G:O2'    | 1:AA:1527:U:H5'   | 2.01                     | 0.60              |
| 12:AM:21:ILE:CG2   | 12:AM:64:VAL:HG11 | 2.30                     | 0.60              |
| 13:AN:24:ALA:O     | 13:AN:27:LYS:HG3  | 2.01                     | 0.60              |
| 18:AS:31:ARG:HG3   | 18:AS:56:HIS:NE2  | 2.15                     | 0.60              |
| 19:AT:68:LYS:HG3   | 19:AT:69:ASN:N    | 2.10                     | 0.60              |
| 20:AB:113:LEU:O    | 20:AB:117:GLU:HG3 | 2.00                     | 0.60              |
| 20:AB:116:LEU:HD11 | 20:AB:139:GLU:HB3 | 1.81                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BB:607:U:OP2   | 27:BE:98:LYS:HG2  | 2.02                     | 0.60              |
| 23:BB:692:C:H5'   | 25:BC:42:ARG:CB   | 2.22                     | 0.60              |
| 23:BB:1439:A:C5   | 23:BB:1552:A:N6   | 2.70                     | 0.60              |
| 23:BB:1810:A:H2'  | 23:BB:1811:G:O4'  | 2.00                     | 0.60              |
| 23:BB:1939:U:O2   | 23:BB:1967:C:H4'  | 2.01                     | 0.60              |
| 23:BB:2599:G:N7   | 25:BC:234:GLY:HA2 | 2.16                     | 0.60              |
| 23:BB:2600:A:H62  | 25:BC:235:GLU:HB3 | 1.66                     | 0.60              |
| 23:BB:2848:G:H2'  | 37:BP:96:LEU:HB2  | 1.83                     | 0.60              |
| 26:BD:31:ALA:HB3  | 26:BD:95:SER:HB3  | 1.84                     | 0.60              |
| 27:BE:106:LYS:HB2 | 27:BE:106:LYS:HZ2 | 1.66                     | 0.60              |
| 30:BH:116:ARG:HB3 | 30:BH:131:SER:OG  | 2.01                     | 0.60              |
| 34:BM:3:GLN:H     | 34:BM:4:PRO:CD    | 1.95                     | 0.60              |
| 35:BN:8:ARG:CZ    | 35:BN:46:ARG:HD2  | 2.32                     | 0.60              |
| 42:BU:13:LEU:H    | 42:BU:68:ASN:ND2  | 2.00                     | 0.60              |
| 1:CA:815:A:H4'    | 1:CA:817:C:C4     | 2.36                     | 0.60              |
| 1:CA:922:G:H2'    | 1:CA:923:A:H8     | 1.66                     | 0.60              |
| 1:CA:1129:C:H1'   | 1:CA:1146:A:H61   | 1.65                     | 0.60              |
| 11:CL:29:LYS:O    | 11:CL:80:LEU:HD12 | 2.01                     | 0.60              |
| 12:CM:15:VAL:HG22 | 12:CM:40:GLU:HB2  | 1.83                     | 0.60              |
| 13:CN:79:SER:O    | 13:CN:83:VAL:HG23 | 2.02                     | 0.60              |
| 14:CO:88:ARG:HH11 | 14:CO:88:ARG:HG3  | 1.66                     | 0.60              |
| 15:CP:4:ILE:O     | 15:CP:71:VAL:HG11 | 2.00                     | 0.60              |
| 23:DB:197:A:N6    | 23:DB:2430:A:H2'  | 2.17                     | 0.60              |
| 23:DB:336:C:H5''  | 42:DU:3:LYS:HZ3   | 1.64                     | 0.60              |
| 23:DB:352:A:H3'   | 23:DB:353:C:H6    | 1.66                     | 0.60              |
| 23:DB:850:U:H2'   | 23:DB:851:C:C6    | 2.36                     | 0.60              |
| 23:DB:1810:A:H2'  | 23:DB:1811:G:O4'  | 2.00                     | 0.60              |
| 23:DB:2888:C:H2'  | 23:DB:2889:C:C6   | 2.36                     | 0.60              |
| 27:DE:176:ASP:HB3 | 27:DE:179:SER:OG  | 2.02                     | 0.60              |
| 37:DP:36:LYS:HG2  | 37:DP:37:LYS:H    | 1.67                     | 0.60              |
| 37:DP:70:GLU:HG2  | 37:DP:71:ARG:H    | 1.67                     | 0.60              |
| 48:D1:8:ILE:HD13  | 48:D1:9:LYS:H     | 1.64                     | 0.60              |
| 48:D1:13:SER:HB3  | 48:D1:49:LYS:HZ3  | 1.66                     | 0.60              |
| 51:D4:36:ARG:HH11 | 51:D4:36:ARG:HG2  | 1.66                     | 0.60              |
| 1:AA:57:G:H2'     | 1:AA:58:C:C6      | 2.36                     | 0.60              |
| 1:AA:74:A:O2'     | 1:AA:75:G:H5''    | 2.02                     | 0.60              |
| 1:AA:769:G:H4'    | 1:AA:1513:A:H4'   | 1.82                     | 0.60              |
| 1:AA:1074:G:H5'   | 20:AB:104:LYS:HZ1 | 1.66                     | 0.60              |
| 1:AA:1320:C:H5    | 18:AS:36:ARG:HG2  | 1.65                     | 0.60              |
| 3:AD:185:PRO:HB2  | 3:AD:190:LEU:HD11 | 1.81                     | 0.60              |
| 4:AE:33:THR:O     | 4:AE:34:ALA:HB3   | 2.00                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:AH:9:MET:HE1    | 7:AH:32:LYS:O     | 2.02                     | 0.60              |
| 7:AH:26:MET:HB2   | 7:AH:27:PRO:HD2   | 1.84                     | 0.60              |
| 8:AI:110:VAL:HG12 | 8:AI:111:GLU:N    | 2.16                     | 0.60              |
| 16:AQ:59:GLU:H    | 16:AQ:74:LEU:HD23 | 1.67                     | 0.60              |
| 22:BA:98:G:H1     | 24:BV:14:LYS:CB   | 2.15                     | 0.60              |
| 23:BB:2331:G:H4'  | 43:BW:69:GLU:CG   | 2.31                     | 0.60              |
| 25:BC:68:ARG:HD3  | 25:BC:103:ILE:CD1 | 2.31                     | 0.60              |
| 33:BL:91:ASP:O    | 33:BL:92:LEU:CB   | 2.49                     | 0.60              |
| 38:BQ:27:ARG:HG3  | 38:BQ:32:ARG:NH2  | 2.16                     | 0.60              |
| 38:BQ:88:GLU:HA   | 39:BR:53:PHE:CE2  | 2.35                     | 0.60              |
| 38:BQ:92:LYS:O    | 38:BQ:94:LEU:N    | 2.34                     | 0.60              |
| 47:B0:36:LYS:HG3  | 47:B0:41:HIS:HA   | 1.83                     | 0.60              |
| 1:CA:60:A:O2'     | 1:CA:61:G:O5'     | 2.19                     | 0.60              |
| 1:CA:403:C:O2'    | 1:CA:404:G:H5'    | 2.01                     | 0.60              |
| 4:CE:36:THR:HG22  | 4:CE:37:VAL:N     | 2.14                     | 0.60              |
| 4:CE:91:SER:HA    | 4:CE:128:GLY:O    | 2.02                     | 0.60              |
| 5:CF:42:TRP:HE1   | 5:CF:61:LEU:HD23  | 1.67                     | 0.60              |
| 13:CN:27:LYS:O    | 13:CN:31:SER:HB3  | 2.00                     | 0.60              |
| 23:DB:448:U:H3'   | 27:DE:79:ARG:NH2  | 2.15                     | 0.60              |
| 23:DB:2679:A:O2'  | 23:DB:2680:U:H5'  | 2.02                     | 0.60              |
| 23:DB:2800:A:H2'  | 23:DB:2801:G:C1'  | 2.32                     | 0.60              |
| 26:DD:107:VAL:HA  | 26:DD:205:PRO:O   | 2.01                     | 0.60              |
| 31:DJ:36:LEU:HA   | 31:DJ:51:GLY:O    | 2.02                     | 0.60              |
| 44:DX:44:LYS:CG   | 44:DX:47:ARG:HB2  | 2.31                     | 0.60              |
| 45:DY:6:ILE:CG1   | 45:DY:35:VAL:H    | 2.13                     | 0.60              |
| 52:DI:125:THR:O   | 52:DI:129:GLU:HG3 | 2.01                     | 0.60              |
| 1:AA:859:G:H2'    | 1:AA:860:A:H8     | 1.65                     | 0.60              |
| 2:AC:58:ARG:CG    | 2:AC:63:ILE:HG22  | 2.31                     | 0.60              |
| 3:AD:150:LYS:HB2  | 3:AD:150:LYS:NZ   | 2.17                     | 0.60              |
| 10:AK:52:ARG:HD2  | 10:AK:53:GLY:H    | 1.67                     | 0.60              |
| 23:BB:328:U:H4'   | 42:BU:65:GLN:NE2  | 2.16                     | 0.60              |
| 23:BB:926:G:H2'   | 23:BB:927:A:H8    | 1.66                     | 0.60              |
| 23:BB:1805:A:N3   | 25:BC:50:THR:HG23 | 2.16                     | 0.60              |
| 23:BB:1878:G:H2'  | 23:BB:1879:C:C6   | 2.37                     | 0.60              |
| 23:BB:2642:G:O2'  | 23:BB:2643:G:H5'  | 2.01                     | 0.60              |
| 23:BB:2679:A:O2'  | 23:BB:2680:U:H5'  | 2.02                     | 0.60              |
| 23:BB:2698:U:H2'  | 23:BB:2699:C:C6   | 2.37                     | 0.60              |
| 23:BB:2769:U:H2'  | 23:BB:2770:G:C8   | 2.36                     | 0.60              |
| 24:BV:46:LYS:HA   | 24:BV:46:LYS:HE3  | 1.84                     | 0.60              |
| 25:BC:30:ALA:N    | 25:BC:31:PRO:HD3  | 2.09                     | 0.60              |
| 32:BK:2:ILE:HG22  | 32:BK:67:LYS:NZ   | 2.16                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:BL:77:ILE:CG2   | 33:BL:78:ARG:HG3   | 2.32                     | 0.60              |
| 34:BM:58:LYS:C     | 34:BM:60:GLN:H     | 2.07                     | 0.60              |
| 39:BR:74:ILE:CA    | 39:BR:90:ARG:HE    | 2.10                     | 0.60              |
| 42:BU:85:ARG:HD3   | 42:BU:85:ARG:N     | 2.17                     | 0.60              |
| 48:B1:5:ARG:HH11   | 48:B1:5:ARG:HB3    | 1.65                     | 0.60              |
| 1:CA:994:A:C5      | 1:CA:1216:A:H4'    | 2.36                     | 0.60              |
| 3:CD:171:GLU:HG3   | 3:CD:182:LYS:HD2   | 1.83                     | 0.60              |
| 4:CE:113:VAL:HG23  | 4:CE:114:LEU:H     | 1.66                     | 0.60              |
| 20:CB:16:GLY:HA2   | 20:CB:40:ILE:H     | 1.66                     | 0.60              |
| 22:DA:35:C:O2'     | 22:DA:36:C:H5'     | 2.02                     | 0.60              |
| 23:DB:990:A:N6     | 23:DB:1186:G:H1'   | 2.17                     | 0.60              |
| 23:DB:1082:U:O4    | 23:DB:1086:A:C2    | 2.55                     | 0.60              |
| 23:DB:1203:U:H3'   | 23:DB:1204:A:C5'   | 2.31                     | 0.60              |
| 23:DB:1439:A:C5    | 23:DB:1552:A:N6    | 2.70                     | 0.60              |
| 23:DB:1791:A:C2    | 23:DB:1829:A:H4'   | 2.36                     | 0.60              |
| 23:DB:2090:A:O2'   | 46:DZ:49:ARG:HD2   | 2.02                     | 0.60              |
| 23:DB:2360:G:H1'   | 33:DL:61:LEU:HD11  | 1.82                     | 0.60              |
| 23:DB:2887:A:C8    | 47:D0:27:LEU:HD21  | 2.36                     | 0.60              |
| 26:DD:24:VAL:HG13  | 26:DD:193:VAL:HG21 | 1.84                     | 0.60              |
| 27:DE:157:LEU:HD23 | 27:DE:157:LEU:H    | 1.66                     | 0.60              |
| 31:DJ:25:LEU:CD1   | 31:DJ:63:ALA:H     | 2.14                     | 0.60              |
| 32:DK:9:ASN:O      | 32:DK:10:VAL:HG13  | 2.01                     | 0.60              |
| 33:DL:38:GLN:NE2   | 33:DL:39:LYS:HE2   | 2.16                     | 0.60              |
| 35:DN:56:LYS:CG    | 35:DN:57:THR:H     | 2.14                     | 0.60              |
| 37:DP:48:ALA:O     | 37:DP:49:ILE:HG22  | 2.01                     | 0.60              |
| 41:DT:88:LYS:HG3   | 41:DT:89:GLU:OE1   | 2.02                     | 0.60              |
| 42:DU:78:LYS:HD2   | 42:DU:96:LYS:HG3   | 1.83                     | 0.60              |
| 1:AA:812:G:O2'     | 1:AA:813:U:H6      | 1.85                     | 0.60              |
| 1:AA:812:G:HO2'    | 1:AA:813:U:H6      | 1.49                     | 0.60              |
| 5:AF:46:GLN:HA     | 5:AF:56:LYS:HG3    | 1.81                     | 0.60              |
| 5:AF:61:LEU:HD12   | 5:AF:63:ASN:OD1    | 2.02                     | 0.60              |
| 13:AN:15:LEU:HD12  | 13:AN:16:ALA:H     | 1.66                     | 0.60              |
| 16:AQ:60:ILE:N     | 16:AQ:60:ILE:HD13  | 2.16                     | 0.60              |
| 23:BB:26:G:H1'     | 23:BB:514:A:N6     | 2.17                     | 0.60              |
| 23:BB:176:A:O2'    | 23:BB:177:G:H5'    | 2.01                     | 0.60              |
| 23:BB:418:C:H2'    | 23:BB:419:U:C6     | 2.36                     | 0.60              |
| 23:BB:433:C:H2'    | 23:BB:434:U:C6     | 2.37                     | 0.60              |
| 23:BB:836:G:H2'    | 23:BB:837:C:C6     | 2.37                     | 0.60              |
| 23:BB:910:A:N7     | 34:BM:16:ARG:HB2   | 2.17                     | 0.60              |
| 23:BB:997:G:H5'    | 38:BQ:91:ARG:HG3   | 1.83                     | 0.60              |
| 23:BB:1791:A:N6    | 23:BB:1828:G:H1'   | 2.16                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:2650:U:H2'  | 23:BB:2651:C:C6    | 2.35                     | 0.60              |
| 23:BB:2671:G:H2'  | 23:BB:2672:U:C6    | 2.37                     | 0.60              |
| 25:BC:58:LYS:O    | 25:BC:59:GLN:HG3   | 2.02                     | 0.60              |
| 28:BF:174:PHE:N   | 28:BF:175:PRO:CD   | 2.63                     | 0.60              |
| 33:BL:60:ARG:HD2  | 50:B3:7:ARG:HE     | 1.66                     | 0.60              |
| 37:BP:50:ARG:HH11 | 37:BP:50:ARG:CB    | 2.09                     | 0.60              |
| 39:BR:85:LYS:C    | 39:BR:87:GLN:H     | 2.09                     | 0.60              |
| 40:BS:29:VAL:HG22 | 40:BS:71:VAL:HG23  | 1.83                     | 0.60              |
| 44:BX:44:LYS:O    | 44:BX:48:ARG:HD2   | 2.02                     | 0.60              |
| 1:CA:590:U:H2'    | 1:CA:591:U:H6      | 1.67                     | 0.60              |
| 1:CA:1124:G:H5'   | 9:CJ:37:ARG:NH2    | 2.17                     | 0.60              |
| 1:CA:1256:A:N1    | 1:CA:1278:G:H1'    | 2.16                     | 0.60              |
| 2:CC:11:LEU:HD22  | 2:CC:17:TRP:NE1    | 2.17                     | 0.60              |
| 2:CC:56:ILE:HD12  | 2:CC:56:ILE:N      | 2.16                     | 0.60              |
| 4:CE:142:GLY:HA2  | 4:CE:145:ASN:ND2   | 2.16                     | 0.60              |
| 5:CF:36:ILE:HG12  | 5:CF:64:VAL:HG22   | 1.83                     | 0.60              |
| 13:CN:30:ILE:CG2  | 13:CN:41:TRP:HB3   | 2.31                     | 0.60              |
| 23:DB:1857:G:H2'  | 23:DB:1884:G:H22   | 1.66                     | 0.60              |
| 23:DB:1878:G:H2'  | 23:DB:1879:C:C6    | 2.37                     | 0.60              |
| 23:DB:1915:U:H2'  | 23:DB:1916:A:O4'   | 2.02                     | 0.60              |
| 23:DB:1939:U:O2   | 23:DB:1967:C:H4'   | 2.01                     | 0.60              |
| 25:DC:92:LEU:O    | 25:DC:93:VAL:HB    | 2.01                     | 0.60              |
| 25:DC:205:GLY:C   | 25:DC:206:LYS:HG2  | 2.27                     | 0.60              |
| 26:DD:129:THR:HA  | 26:DD:140:HIS:CE1  | 2.36                     | 0.60              |
| 33:DL:91:ASP:O    | 33:DL:93:ASN:N     | 2.33                     | 0.60              |
| 34:DM:29:GLY:N    | 34:DM:102:LEU:HD12 | 2.12                     | 0.60              |
| 34:DM:73:ILE:HG21 | 34:DM:90:GLU:CD    | 2.27                     | 0.60              |
| 35:DN:54:LEU:HD23 | 35:DN:54:LEU:O     | 2.02                     | 0.60              |
| 41:DT:61:LEU:HB2  | 41:DT:82:LYS:HB3   | 1.83                     | 0.60              |
| 1:AA:26:A:H61     | 1:AA:558:G:H1'     | 1.65                     | 0.60              |
| 1:AA:51:A:O2'     | 1:AA:52:C:OP2      | 2.18                     | 0.60              |
| 1:AA:56:U:H2'     | 1:AA:57:G:C8       | 2.36                     | 0.60              |
| 1:AA:590:U:H2'    | 1:AA:591:U:H6      | 1.66                     | 0.60              |
| 4:AE:85:LYS:HE3   | 4:AE:94:PHE:HB2    | 1.84                     | 0.60              |
| 4:AE:109:ALA:HB3  | 4:AE:135:VAL:HG23  | 1.82                     | 0.60              |
| 7:AH:92:PRO:HA    | 7:AH:93:LYS:HZ2    | 1.66                     | 0.60              |
| 8:AI:49:GLN:HE21  | 8:AI:79:ARG:HD2    | 1.67                     | 0.60              |
| 17:AR:46:THR:HG23 | 17:AR:51:GLN:HB2   | 1.81                     | 0.60              |
| 20:AB:46:VAL:CG1  | 20:AB:47:PRO:HD3   | 2.25                     | 0.60              |
| 23:BB:27:G:H1'    | 23:BB:513:A:N6     | 2.17                     | 0.60              |
| 23:BB:575:A:O2'   | 23:BB:576:U:H5'    | 2.02                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:1729:U:C5    | 23:BB:1730:C:H1'   | 2.37                     | 0.60              |
| 23:BB:2050:C:H4'   | 26:BD:143:PRO:HG2  | 1.84                     | 0.60              |
| 25:BC:224:MET:HE3  | 25:BC:232:GLY:C    | 2.27                     | 0.60              |
| 26:BD:153:GLY:O    | 26:BD:154:LYS:HB2  | 2.01                     | 0.60              |
| 30:BH:6:LEU:HA     | 30:BH:15:LEU:HA    | 1.83                     | 0.60              |
| 33:BL:126:ARG:O    | 33:BL:127:VAL:HG13 | 2.02                     | 0.60              |
| 36:BO:16:ARG:O     | 36:BO:20:GLU:HB2   | 2.01                     | 0.60              |
| 40:BS:24:ILE:HD13  | 40:BS:36:LEU:HD21  | 1.83                     | 0.60              |
| 42:BU:12:VAL:HA    | 42:BU:68:ASN:ND2   | 2.12                     | 0.60              |
| 1:CA:135:C:O2      | 15:CP:1:MET:HB2    | 2.02                     | 0.60              |
| 1:CA:1118:U:H2'    | 1:CA:1119:C:H6     | 1.67                     | 0.60              |
| 1:CA:1320:C:OP2    | 18:CS:2:ARG:HB3    | 2.02                     | 0.60              |
| 2:CC:110:LEU:HD13  | 2:CC:143:LEU:HD23  | 1.83                     | 0.60              |
| 4:CE:158:LYS:CB    | 7:CH:63:LYS:HD3    | 2.30                     | 0.60              |
| 6:CG:49:LEU:C      | 6:CG:51:GLN:H      | 2.07                     | 0.60              |
| 13:CN:30:ILE:HB    | 13:CN:44:VAL:HB    | 1.83                     | 0.60              |
| 18:CS:27:LYS:HB3   | 18:CS:27:LYS:NZ    | 2.17                     | 0.60              |
| 23:DB:717:C:C3'    | 23:DB:718:A:H5''   | 2.30                     | 0.60              |
| 23:DB:1164:C:H2'   | 23:DB:1165:A:H8    | 1.65                     | 0.60              |
| 23:DB:2868:A:H2'   | 23:DB:2869:G:C8    | 2.37                     | 0.60              |
| 25:DC:257:ARG:HH11 | 25:DC:257:ARG:HG2  | 1.66                     | 0.60              |
| 26:DD:18:ASP:C     | 26:DD:20:VAL:H     | 2.10                     | 0.60              |
| 34:DM:41:LEU:HB3   | 34:DM:93:VAL:HB    | 1.83                     | 0.60              |
| 37:DP:25:VAL:C     | 37:DP:27:VAL:H     | 2.10                     | 0.60              |
| 37:DP:106:ALA:O    | 37:DP:108:ARG:HD2  | 2.01                     | 0.60              |
| 38:DQ:98:ALA:HA    | 38:DQ:105:PHE:CD1  | 2.36                     | 0.60              |
| 46:DZ:1:MET:HA     | 46:DZ:9:TYR:CD1    | 2.37                     | 0.60              |
| 46:DZ:30:HIS:O     | 46:DZ:48:GLN:HA    | 2.01                     | 0.60              |
| 52:DI:63:ASP:O     | 52:DI:64:ARG:HB2   | 2.00                     | 0.60              |
| 1:AA:34:C:H2'      | 1:AA:35:G:H8       | 1.67                     | 0.60              |
| 1:AA:865:A:H2'     | 1:AA:866:C:H6      | 1.67                     | 0.60              |
| 1:AA:987:G:H2'     | 1:AA:988:G:C8      | 2.35                     | 0.60              |
| 2:AC:5:HIS:CD2     | 2:AC:8:GLY:H       | 2.19                     | 0.60              |
| 5:AF:37:HIS:CE1    | 5:AF:65:GLU:HB2    | 2.36                     | 0.60              |
| 8:AI:18:VAL:HG22   | 8:AI:64:ILE:HG23   | 1.84                     | 0.60              |
| 12:AM:103:THR:HG22 | 12:AM:104:ASN:H    | 1.67                     | 0.60              |
| 20:AB:162:VAL:HG13 | 20:AB:184:ALA:HB2  | 1.83                     | 0.60              |
| 23:BB:1082:U:O4    | 23:BB:1086:A:C2    | 2.55                     | 0.60              |
| 23:BB:1655:A:C2    | 23:BB:2049:G:H5''  | 2.36                     | 0.60              |
| 23:BB:2053:G:OP1   | 26:BD:149:ASN:C    | 2.44                     | 0.60              |
| 23:BB:2674:G:H4'   | 32:BK:30:ARG:CG    | 2.31                     | 0.60              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:BC:32:LEU:HD13 | 25:BC:61:TYR:HE1   | 1.67                     | 0.60              |
| 26:BD:5:VAL:HG11  | 26:BD:28:GLU:CA    | 2.31                     | 0.60              |
| 31:BJ:90:GLU:O    | 31:BJ:93:ILE:HG22  | 2.02                     | 0.60              |
| 33:BL:39:LYS:HB2  | 33:BL:46:VAL:HA    | 1.83                     | 0.60              |
| 33:BL:83:ALA:N    | 33:BL:86:GLU:HG3   | 2.15                     | 0.60              |
| 51:B4:24:ARG:HH12 | 51:B4:36:ARG:HB2   | 1.66                     | 0.60              |
| 1:CA:160:A:H2'    | 1:CA:161:A:O4'     | 2.00                     | 0.60              |
| 1:CA:1513:A:H2'   | 1:CA:1514:G:C8     | 2.37                     | 0.60              |
| 4:CE:19:ARG:HG2   | 4:CE:20:VAL:N      | 2.15                     | 0.60              |
| 7:CH:75:GLN:NE2   | 7:CH:76:ARG:H      | 1.99                     | 0.60              |
| 18:CS:18:VAL:HG22 | 18:CS:42:ASN:ND2   | 2.17                     | 0.60              |
| 20:CB:187:ASP:HB3 | 20:CB:201:GLY:O    | 2.02                     | 0.60              |
| 23:DB:138:U:H2'   | 23:DB:140:C:O4'    | 2.01                     | 0.60              |
| 23:DB:992:C:H4'   | 38:DQ:46:TYR:OH    | 2.01                     | 0.60              |
| 23:DB:2386:A:H2'  | 23:DB:2387:U:C6    | 2.37                     | 0.60              |
| 23:DB:2698:U:H2'  | 23:DB:2699:C:C6    | 2.36                     | 0.60              |
| 24:DV:77:VAL:HG13 | 24:DV:89:ILE:HD11  | 1.82                     | 0.60              |
| 26:DD:37:VAL:HG13 | 26:DD:42:ASN:CB    | 2.31                     | 0.60              |
| 27:DE:76:PRO:HA   | 27:DE:82:GLY:O     | 2.02                     | 0.60              |
| 27:DE:105:LEU:H   | 27:DE:105:LEU:HD22 | 1.67                     | 0.60              |
| 29:DG:138:GLN:NE2 | 29:DG:142:GLN:HG3  | 2.17                     | 0.60              |
| 31:DJ:85:LYS:HE2  | 31:DJ:85:LYS:HA    | 1.83                     | 0.60              |
| 37:DP:47:ILE:CG2  | 37:DP:63:ILE:HA    | 2.28                     | 0.60              |
| 37:DP:47:ILE:CG1  | 37:DP:63:ILE:HG23  | 2.26                     | 0.60              |
| 48:D1:22:THR:O    | 48:D1:23:THR:C     | 2.44                     | 0.60              |
| 1:AA:238:A:C2'    | 1:AA:239:U:H5''    | 2.31                     | 0.60              |
| 1:AA:1458:G:H5'   | 19:AT:26:MET:HB2   | 1.84                     | 0.60              |
| 10:AK:86:LYS:HD2  | 10:AK:114:PRO:HD3  | 1.84                     | 0.60              |
| 11:AL:85:ARG:HA   | 11:AL:93:ARG:HA    | 1.84                     | 0.60              |
| 22:BA:39:A:O2'    | 22:BA:40:U:H5'     | 2.01                     | 0.60              |
| 22:BA:75:G:H5''   | 24:BV:12:GLN:OE1   | 2.01                     | 0.60              |
| 23:BB:634:C:H2'   | 23:BB:635:C:C6     | 2.37                     | 0.60              |
| 23:BB:651:G:H4'   | 50:B3:17:GLY:HA3   | 1.84                     | 0.60              |
| 23:BB:864:G:O2'   | 23:BB:865:C:H5'    | 2.02                     | 0.60              |
| 23:BB:1454:C:C5'  | 35:BN:63:ARG:HH21  | 2.06                     | 0.60              |
| 23:BB:1557:C:H3'  | 23:BB:1558:C:H5''  | 1.84                     | 0.60              |
| 23:BB:2811:G:C5'  | 26:BD:62:LYS:HD2   | 2.31                     | 0.60              |
| 24:BV:26:PHE:HE2  | 24:BV:44:HIS:HA    | 1.66                     | 0.60              |
| 28:BF:64:PRO:HA   | 28:BF:88:VAL:CG2   | 2.32                     | 0.60              |
| 30:BH:21:VAL:HG22 | 30:BH:22:LYS:N     | 2.13                     | 0.60              |
| 33:BL:27:LEU:C    | 33:BL:29:LYS:H     | 2.10                     | 0.60              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:BL:120:VAL:HG22 | 33:BL:122:VAL:HG13 | 1.83                     | 0.60              |
| 35:BN:107:ASN:OD1  | 40:BS:40:ASN:HB3   | 2.01                     | 0.60              |
| 38:BQ:94:LEU:HD22  | 38:BQ:95:ALA:N     | 2.16                     | 0.60              |
| 41:BT:24:MET:CE    | 41:BT:29:THR:H     | 2.15                     | 0.60              |
| 42:BU:42:LYS:HD3   | 42:BU:60:LYS:HB3   | 1.83                     | 0.60              |
| 49:B2:17:GLY:HA2   | 49:B2:21:ARG:NH1   | 2.17                     | 0.60              |
| 49:B2:34:ARG:HE    | 49:B2:42:LEU:CD1   | 2.14                     | 0.60              |
| 1:CA:254:G:OP1     | 16:CQ:68:LYS:O     | 2.20                     | 0.60              |
| 1:CA:599:C:H5''    | 7:CH:86:LYS:O      | 2.02                     | 0.60              |
| 1:CA:1038:C:H2'    | 1:CA:1039:G:C8     | 2.36                     | 0.60              |
| 7:CH:86:LYS:HB3    | 7:CH:90:GLU:O      | 2.02                     | 0.60              |
| 9:CJ:22:THR:O      | 9:CJ:26:VAL:HG23   | 2.01                     | 0.60              |
| 9:CJ:42:LEU:HB3    | 9:CJ:43:PRO:HD2    | 1.84                     | 0.60              |
| 12:CM:52:ILE:HD12  | 12:CM:55:LEU:HD12  | 1.83                     | 0.60              |
| 13:CN:62:ARG:HH21  | 13:CN:69:PRO:HG3   | 1.65                     | 0.60              |
| 23:DB:1429:G:H2'   | 23:DB:1430:G:C8    | 2.37                     | 0.60              |
| 23:DB:1484:U:H2'   | 23:DB:1485:U:C6    | 2.37                     | 0.60              |
| 23:DB:2010:G:H5''  | 40:DS:42:LYS:CB    | 2.31                     | 0.60              |
| 23:DB:2241:A:H2'   | 23:DB:2242:G:C8    | 2.36                     | 0.60              |
| 23:DB:2671:G:H2'   | 23:DB:2672:U:C6    | 2.36                     | 0.60              |
| 44:DX:58:ASN:ND2   | 44:DX:63:ALA:HB3   | 2.16                     | 0.60              |
| 45:DY:18:LYS:O     | 45:DY:22:THR:HG23  | 2.02                     | 0.60              |
| 52:DI:11:GLN:HA    | 52:DI:55:PRO:HA    | 1.83                     | 0.60              |
| 1:AA:320:A:H2'     | 1:AA:321:A:C8      | 2.37                     | 0.59              |
| 1:AA:1035:A:H2'    | 1:AA:1036:A:C8     | 2.36                     | 0.59              |
| 3:AD:58:GLN:HA     | 3:AD:61:ARG:HB2    | 1.84                     | 0.59              |
| 3:AD:194:ILE:HD13  | 3:AD:195:ASN:H     | 1.67                     | 0.59              |
| 16:AQ:24:ILE:HB    | 16:AQ:41:THR:HB    | 1.82                     | 0.59              |
| 20:AB:118:THR:O    | 20:AB:121:GLN:HB3  | 2.02                     | 0.59              |
| 23:BB:401:A:H2'    | 23:BB:402:A:C8     | 2.37                     | 0.59              |
| 23:BB:624:C:OP1    | 50:B3:61:LEU:HB3   | 2.01                     | 0.59              |
| 23:BB:956:G:N2     | 23:BB:959:A:H3'    | 2.16                     | 0.59              |
| 23:BB:1229:C:H2'   | 23:BB:1230:A:H8    | 1.65                     | 0.59              |
| 23:BB:1295:C:H2'   | 23:BB:1296:G:C8    | 2.36                     | 0.59              |
| 25:BC:61:TYR:CD2   | 25:BC:84:PRO:HD2   | 2.37                     | 0.59              |
| 25:BC:143:VAL:O    | 25:BC:152:GLN:HB2  | 2.01                     | 0.59              |
| 26:BD:35:THR:HG22  | 26:BD:46:ARG:NH2   | 2.16                     | 0.59              |
| 26:BD:49:GLN:O     | 26:BD:78:GLY:HA2   | 2.00                     | 0.59              |
| 27:BE:118:LEU:C    | 27:BE:119:ILE:HD12 | 2.27                     | 0.59              |
| 33:BL:90:VAL:HG11  | 33:BL:121:THR:N    | 2.11                     | 0.59              |
| 41:BT:64:LYS:NZ    | 41:BT:79:ASP:HB2   | 2.17                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:22:G:H4'      | 1:CA:885:G:C8      | 2.37                     | 0.59              |
| 1:CA:77:A:H2'      | 1:CA:78:A:C8       | 2.36                     | 0.59              |
| 1:CA:320:A:H2'     | 1:CA:321:A:C8      | 2.37                     | 0.59              |
| 1:CA:742:G:O2'     | 1:CA:743:A:H5'     | 2.02                     | 0.59              |
| 1:CA:1021:A:H2'    | 1:CA:1022:A:O4'    | 2.02                     | 0.59              |
| 1:CA:1355:G:H2'    | 1:CA:1356:G:H8     | 1.67                     | 0.59              |
| 3:CD:101:VAL:HG13  | 3:CD:106:PHE:CD2   | 2.34                     | 0.59              |
| 4:CE:28:ARG:HH22   | 4:CE:30:PHE:HB3    | 1.67                     | 0.59              |
| 4:CE:152:VAL:HG21  | 7:CH:98:LEU:HB3    | 1.82                     | 0.59              |
| 7:CH:31:LEU:O      | 7:CH:35:ILE:HG13   | 2.01                     | 0.59              |
| 7:CH:76:ARG:HE     | 7:CH:125:ILE:HG23  | 1.67                     | 0.59              |
| 12:CM:44:ILE:C     | 12:CM:44:ILE:HD12  | 2.27                     | 0.59              |
| 13:CN:26:LEU:HD12  | 13:CN:29:ILE:HD12  | 1.83                     | 0.59              |
| 15:CP:54:LEU:HD13  | 15:CP:80:LYS:HZ2   | 1.67                     | 0.59              |
| 19:CT:66:ILE:O     | 19:CT:70:LYS:HD3   | 2.02                     | 0.59              |
| 23:DB:322:A:H1'    | 23:DB:339:U:O2     | 2.01                     | 0.59              |
| 23:DB:493:G:H2'    | 23:DB:494:G:O4'    | 2.01                     | 0.59              |
| 23:DB:858:G:H21    | 23:DB:2268:A:H3'   | 1.67                     | 0.59              |
| 23:DB:1387:A:H5'   | 23:DB:1469:A:H1'   | 1.84                     | 0.59              |
| 23:DB:1474:U:H2'   | 23:DB:1475:G:H5'   | 1.83                     | 0.59              |
| 23:DB:2617:U:H2'   | 23:DB:2618:G:H5'   | 1.84                     | 0.59              |
| 23:DB:2769:U:H2'   | 23:DB:2770:G:C8    | 2.36                     | 0.59              |
| 25:DC:143:VAL:HG11 | 25:DC:173:LEU:HD11 | 1.84                     | 0.59              |
| 26:DD:125:TRP:HB2  | 26:DD:160:LYS:HD3  | 1.84                     | 0.59              |
| 27:DE:187:VAL:HG23 | 27:DE:188:MET:N    | 2.17                     | 0.59              |
| 30:DH:26:ALA:C     | 30:DH:28:ASN:N     | 2.60                     | 0.59              |
| 30:DH:124:THR:HG23 | 30:DH:128:HIS:NE2  | 2.17                     | 0.59              |
| 32:DK:11:ALA:HB1   | 32:DK:100:PHE:O    | 2.01                     | 0.59              |
| 49:D2:35:ARG:NH2   | 49:D2:44:VAL:HG22  | 2.17                     | 0.59              |
| 1:AA:1103:C:H5''   | 20:AB:96:LEU:HD12  | 1.82                     | 0.59              |
| 1:AA:1137:C:H1'    | 1:AA:1138:G:N2     | 2.16                     | 0.59              |
| 23:BB:28:A:N6      | 23:BB:512:G:H1'    | 2.17                     | 0.59              |
| 23:BB:1285:A:H2'   | 23:BB:1286:A:H5''  | 1.83                     | 0.59              |
| 23:BB:1550:C:H2'   | 23:BB:1551:A:H8    | 1.67                     | 0.59              |
| 23:BB:2226:C:H2'   | 23:BB:2227:A:O4'   | 2.02                     | 0.59              |
| 23:BB:2859:G:H2'   | 23:BB:2860:A:C8    | 2.36                     | 0.59              |
| 24:BV:14:LYS:NZ    | 24:BV:18:ARG:HD2   | 2.18                     | 0.59              |
| 25:BC:77:VAL:HG23  | 25:BC:115:ILE:CD1  | 2.31                     | 0.59              |
| 25:BC:128:THR:HG22 | 25:BC:188:ARG:HB2  | 1.84                     | 0.59              |
| 28:BF:132:ARG:CZ   | 28:BF:147:ARG:HE   | 2.15                     | 0.59              |
| 30:BH:125:THR:CB   | 30:BH:146:VAL:HB   | 2.31                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BJ:28:LEU:HG    | 31:BJ:32:LEU:HD13  | 1.84                     | 0.59              |
| 34:BM:102:LEU:HB3  | 34:BM:104:GLU:OE2  | 2.02                     | 0.59              |
| 35:BN:1:MET:HE3    | 35:BN:3:HIS:H      | 1.66                     | 0.59              |
| 35:BN:96:ARG:NH2   | 35:BN:118:ARG:HB3  | 2.17                     | 0.59              |
| 37:BP:30:TRP:HB2   | 37:BP:82:SER:OG    | 2.01                     | 0.59              |
| 46:BZ:5:ILE:HD13   | 46:BZ:47:LYS:HB3   | 1.82                     | 0.59              |
| 1:CA:1095:U:H2'    | 1:CA:1096:C:C6     | 2.37                     | 0.59              |
| 6:CG:2:ARG:HB3     | 6:CG:2:ARG:HH11    | 1.66                     | 0.59              |
| 13:CN:51:PRO:HB2   | 13:CN:54:SER:HB3   | 1.84                     | 0.59              |
| 23:DB:575:A:O2'    | 23:DB:576:U:H5'    | 2.02                     | 0.59              |
| 23:DB:969:G:H2'    | 23:DB:970:U:H6     | 1.66                     | 0.59              |
| 23:DB:1729:U:C5    | 23:DB:1730:C:H1'   | 2.37                     | 0.59              |
| 23:DB:1799:G:OP1   | 25:DC:255:LYS:HG2  | 2.02                     | 0.59              |
| 23:DB:1874:C:H2'   | 23:DB:1875:G:O4'   | 2.01                     | 0.59              |
| 29:DG:19:ASN:HB3   | 29:DG:22:VAL:HB    | 1.84                     | 0.59              |
| 30:DH:2:GLN:HA     | 30:DH:21:VAL:HG13  | 1.82                     | 0.59              |
| 35:DN:96:ARG:O     | 35:DN:113:ILE:HA   | 2.01                     | 0.59              |
| 36:DO:50:ALA:HB1   | 36:DO:78:VAL:HG13  | 1.82                     | 0.59              |
| 37:DP:18:SER:HB2   | 37:DP:87:ARG:CZ    | 2.31                     | 0.59              |
| 37:DP:25:VAL:HG22  | 37:DP:89:GLY:N     | 2.15                     | 0.59              |
| 40:DS:21:ALA:HB1   | 40:DS:74:ILE:CD1   | 2.32                     | 0.59              |
| 40:DS:85:ILE:HD11  | 40:DS:93:ALA:HB1   | 1.82                     | 0.59              |
| 43:DW:46:ALA:HB2   | 43:DW:75:ASN:O     | 2.02                     | 0.59              |
| 43:DW:48:ALA:HA    | 43:DW:54:ARG:H     | 1.67                     | 0.59              |
| 48:D1:13:SER:HB3   | 48:D1:49:LYS:NZ    | 2.17                     | 0.59              |
| 8:AI:53:LEU:O      | 8:AI:53:LEU:HD13   | 2.02                     | 0.59              |
| 23:BB:143:C:H3'    | 23:BB:144:A:C8     | 2.37                     | 0.59              |
| 23:BB:660:C:H2'    | 23:BB:661:A:H8     | 1.68                     | 0.59              |
| 23:BB:672:C:O2'    | 23:BB:673:C:H5'    | 2.03                     | 0.59              |
| 23:BB:2273:A:H2'   | 23:BB:2274:A:C8    | 2.37                     | 0.59              |
| 23:BB:2339:C:H2'   | 23:BB:2340:A:C8    | 2.37                     | 0.59              |
| 23:BB:2539:C:OP1   | 51:B4:4:ARG:HD2    | 2.02                     | 0.59              |
| 27:BE:149:ILE:HG13 | 27:BE:186:VAL:HG13 | 1.84                     | 0.59              |
| 28:BF:132:ARG:HD3  | 28:BF:133:GLU:HB2  | 1.84                     | 0.59              |
| 29:BG:157:LYS:HG3  | 29:BG:159:LYS:NZ   | 2.16                     | 0.59              |
| 31:BJ:43:GLU:HB3   | 38:BQ:99:VAL:HG12  | 1.84                     | 0.59              |
| 41:BT:68:LYS:HD3   | 41:BT:68:LYS:C     | 2.28                     | 0.59              |
| 42:BU:48:VAL:HG12  | 42:BU:50:ALA:HB3   | 1.84                     | 0.59              |
| 51:B4:4:ARG:HG2    | 51:B4:4:ARG:O      | 2.02                     | 0.59              |
| 1:CA:202:G:H2'     | 1:CA:203:G:C8      | 2.37                     | 0.59              |
| 4:CE:96:GLN:HG3    | 4:CE:97:PRO:HD2    | 1.84                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:CG:12:LEU:HD13   | 6:CG:13:PRO:CD     | 2.31                     | 0.59              |
| 10:CK:53:GLY:O     | 10:CK:56:LYS:HB3   | 2.02                     | 0.59              |
| 12:CM:10:ASP:HA    | 12:CM:44:ILE:HD11  | 1.83                     | 0.59              |
| 20:CB:96:LEU:O     | 20:CB:99:MET:HG3   | 2.02                     | 0.59              |
| 23:DB:136:G:N2     | 41:DT:3:ARG:HG2    | 2.17                     | 0.59              |
| 23:DB:585:G:H2'    | 23:DB:1251:C:H42   | 1.66                     | 0.59              |
| 23:DB:1695:G:O2'   | 25:DC:15:VAL:HG23  | 2.02                     | 0.59              |
| 23:DB:1814:G:H4'   | 25:DC:51:ARG:HG2   | 1.83                     | 0.59              |
| 23:DB:2107:G:H2'   | 23:DB:2108:A:H8    | 1.67                     | 0.59              |
| 23:DB:2785:C:H2'   | 23:DB:2786:U:C6    | 2.37                     | 0.59              |
| 23:DB:2789:C:H2'   | 23:DB:2893:A:N7    | 2.17                     | 0.59              |
| 23:DB:2900:A:H2'   | 23:DB:2901:C:H6    | 1.66                     | 0.59              |
| 25:DC:10:PRO:HD2   | 25:DC:202:ARG:NH2  | 2.16                     | 0.59              |
| 27:DE:109:LEU:HD21 | 27:DE:113:VAL:O    | 2.02                     | 0.59              |
| 29:DG:17:LYS:HE2   | 29:DG:24:THR:N     | 2.18                     | 0.59              |
| 30:DH:40:THR:HB    | 46:DZ:58:ASP:OD2   | 2.03                     | 0.59              |
| 30:DH:115:VAL:HB   | 30:DH:132:PHE:CD1  | 2.37                     | 0.59              |
| 32:DK:34:GLY:O     | 32:DK:37:ASP:HB2   | 2.03                     | 0.59              |
| 36:DO:100:HIS:HA   | 36:DO:104:GLN:HE21 | 1.67                     | 0.59              |
| 51:D4:3:VAL:HG12   | 51:D4:4:ARG:N      | 2.07                     | 0.59              |
| 1:AA:532:A:H62     | 2:AC:191:THR:CG2   | 2.16                     | 0.59              |
| 1:AA:1060:U:H2'    | 1:AA:1061:G:C8     | 2.37                     | 0.59              |
| 1:AA:1060:U:C5'    | 9:AJ:53:ILE:HG22   | 2.32                     | 0.59              |
| 1:AA:1452:C:H4'    | 1:AA:1453:G:H5''   | 1.84                     | 0.59              |
| 3:AD:94:GLU:HA     | 3:AD:103:ARG:HH22  | 1.66                     | 0.59              |
| 9:AJ:26:VAL:O      | 9:AJ:30:LYS:HB3    | 2.02                     | 0.59              |
| 19:AT:43:LYS:HG2   | 19:AT:44:ALA:N     | 2.17                     | 0.59              |
| 23:BB:182:A:H2'    | 23:BB:183:C:C6     | 2.37                     | 0.59              |
| 23:BB:354:A:H2'    | 23:BB:355:U:H5''   | 1.83                     | 0.59              |
| 23:BB:503:A:C4'    | 23:BB:504:A:H5'    | 2.31                     | 0.59              |
| 23:BB:634:C:H2'    | 23:BB:635:C:H6     | 1.67                     | 0.59              |
| 23:BB:784:G:O2'    | 23:BB:785:G:H5''   | 2.00                     | 0.59              |
| 23:BB:1054:A:H2'   | 23:BB:1055:G:H8    | 1.66                     | 0.59              |
| 23:BB:2266:A:H4'   | 23:BB:2267:A:C8    | 2.37                     | 0.59              |
| 23:BB:2852:G:H2'   | 23:BB:2853:C:H6    | 1.67                     | 0.59              |
| 23:BB:2868:A:H2'   | 23:BB:2869:G:C8    | 2.37                     | 0.59              |
| 23:BB:2899:A:H2'   | 23:BB:2900:A:C8    | 2.37                     | 0.59              |
| 29:BG:85:LYS:HB2   | 29:BG:164:ALA:HB2  | 1.83                     | 0.59              |
| 32:BK:23:LYS:HG3   | 32:BK:24:VAL:N     | 2.17                     | 0.59              |
| 33:BL:117:THR:HG21 | 33:BL:120:VAL:HB   | 1.83                     | 0.59              |
| 36:BO:15:ARG:HH12  | 36:BO:17:LYS:HD3   | 1.67                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 39:BR:90:ARG:NH2   | 39:BR:92:TRP:HB3  | 2.17                     | 0.59              |
| 44:BX:49:ASP:HB3   | 44:BX:52:ARG:NH2  | 2.17                     | 0.59              |
| 1:CA:203:G:N2      | 1:CA:205:A:H61    | 2.01                     | 0.59              |
| 1:CA:214:C:H2'     | 1:CA:215:C:C6     | 2.38                     | 0.59              |
| 1:CA:621:A:H2'     | 1:CA:622:A:C8     | 2.37                     | 0.59              |
| 1:CA:1329:A:H5''   | 12:CM:25:GLY:N    | 2.16                     | 0.59              |
| 2:CC:129:PHE:HA    | 2:CC:132:ALA:HB3  | 1.84                     | 0.59              |
| 3:CD:115:GLN:HE22  | 3:CD:153:ARG:HH22 | 1.50                     | 0.59              |
| 9:CJ:36:VAL:HG13   | 9:CJ:76:ILE:HD11  | 1.83                     | 0.59              |
| 12:CM:78:ARG:HG3   | 28:DF:111:ARG:HG2 | 1.83                     | 0.59              |
| 23:DB:235:U:H2'    | 23:DB:236:C:H6    | 1.67                     | 0.59              |
| 23:DB:533:G:H21    | 38:DQ:40:LYS:HD2  | 1.67                     | 0.59              |
| 23:DB:534:U:H4'    | 38:DQ:45:ALA:HB2  | 1.83                     | 0.59              |
| 23:DB:544:C:H2'    | 23:DB:545:U:C5    | 2.37                     | 0.59              |
| 23:DB:899:A:H2'    | 23:DB:900:A:O4'   | 2.02                     | 0.59              |
| 23:DB:1285:A:H2'   | 23:DB:1286:A:H5'' | 1.83                     | 0.59              |
| 23:DB:1295:C:H2'   | 23:DB:1296:G:C8   | 2.36                     | 0.59              |
| 23:DB:1469:A:H2'   | 23:DB:1470:A:H8   | 1.63                     | 0.59              |
| 23:DB:1676:A:H2'   | 23:DB:1677:A:O4'  | 2.02                     | 0.59              |
| 25:DC:225:ASN:O    | 25:DC:227:VAL:N   | 2.35                     | 0.59              |
| 27:DE:46:GLN:HE22  | 27:DE:86:ALA:HB3  | 1.68                     | 0.59              |
| 27:DE:49:ARG:C     | 27:DE:51:GLU:H    | 2.09                     | 0.59              |
| 27:DE:169:VAL:HG13 | 27:DE:170:ARG:N   | 2.08                     | 0.59              |
| 32:DK:8:LEU:HD12   | 32:DK:8:LEU:N     | 2.17                     | 0.59              |
| 32:DK:41:ILE:HG13  | 32:DK:42:THR:N    | 2.17                     | 0.59              |
| 34:DM:71:LYS:HB2   | 34:DM:72:PRO:CD   | 2.32                     | 0.59              |
| 35:DN:32:GLU:HG3   | 35:DN:33:ILE:N    | 2.17                     | 0.59              |
| 39:DR:92:TRP:O     | 39:DR:93:PHE:HB2  | 2.01                     | 0.59              |
| 1:AA:131:A:H2'     | 1:AA:132:C:H6     | 1.68                     | 0.59              |
| 1:AA:1055:A:H4'    | 2:AC:160:GLU:CG   | 2.32                     | 0.59              |
| 1:AA:1101:A:O2'    | 1:AA:1102:A:OP2   | 2.21                     | 0.59              |
| 3:AD:7:LYS:HE3     | 3:AD:7:LYS:HA     | 1.85                     | 0.59              |
| 13:AN:11:LYS:HA    | 13:AN:11:LYS:HZ2  | 1.67                     | 0.59              |
| 13:AN:20:PHE:HA    | 13:AN:24:ALA:HB2  | 1.84                     | 0.59              |
| 15:AP:4:ILE:O      | 15:AP:71:VAL:HG11 | 2.02                     | 0.59              |
| 20:AB:18:GLN:O     | 20:AB:37:VAL:HG23 | 2.02                     | 0.59              |
| 21:AU:36:PHE:CB    | 21:AU:40:PRO:HD3  | 2.31                     | 0.59              |
| 23:BB:478:A:H5''   | 23:BB:479:A:OP2   | 2.02                     | 0.59              |
| 23:BB:718:A:H3'    | 23:BB:719:C:H6    | 1.68                     | 0.59              |
| 23:BB:1818:U:OP1   | 25:BC:155:ARG:HA  | 2.03                     | 0.59              |
| 23:BB:2800:A:H2'   | 23:BB:2801:G:C1'  | 2.32                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:2821:A:OP2  | 35:BN:3:HIS:NE2    | 2.36                     | 0.59              |
| 25:BC:242:HIS:N   | 25:BC:243:PRO:CD   | 2.66                     | 0.59              |
| 26:BD:38:LYS:H    | 26:BD:38:LYS:CE    | 2.15                     | 0.59              |
| 29:BG:5:LYS:HB3   | 29:BG:68:ARG:NH2   | 2.17                     | 0.59              |
| 31:BJ:136:GLN:N   | 31:BJ:137:PRO:CD   | 2.66                     | 0.59              |
| 34:BM:33:LEU:HD12 | 34:BM:101:VAL:HG11 | 1.83                     | 0.59              |
| 36:BO:87:ILE:HG13 | 36:BO:88:LYS:N     | 2.16                     | 0.59              |
| 44:BX:23:ARG:HG3  | 44:BX:28:LEU:HG    | 1.84                     | 0.59              |
| 47:B0:39:ARG:HG2  | 47:B0:39:ARG:O     | 2.03                     | 0.59              |
| 51:B4:25:VAL:HB   | 51:B4:33:HIS:C     | 2.26                     | 0.59              |
| 52:BI:62:ALA:C    | 52:BI:64:ARG:H     | 2.10                     | 0.59              |
| 1:CA:1082:A:O2'   | 1:CA:1083:U:H5'    | 2.02                     | 0.59              |
| 1:CA:1137:C:O2'   | 1:CA:1138:G:H5''   | 2.03                     | 0.59              |
| 7:CH:76:ARG:HA    | 7:CH:126:CYS:HB3   | 1.85                     | 0.59              |
| 16:CQ:10:ARG:NH2  | 16:CQ:55:GLY:H     | 2.00                     | 0.59              |
| 16:CQ:14:ASP:OD2  | 16:CQ:53:GLY:HA2   | 2.01                     | 0.59              |
| 23:DB:1097:U:H2'  | 23:DB:1098:A:O4'   | 2.03                     | 0.59              |
| 23:DB:1099:G:C8   | 52:DI:3:LYS:CA     | 2.75                     | 0.59              |
| 23:DB:1945:G:H2'  | 23:DB:1946:U:C6    | 2.38                     | 0.59              |
| 23:DB:2329:U:H2'  | 23:DB:2330:G:C8    | 2.37                     | 0.59              |
| 23:DB:2642:G:O2'  | 23:DB:2643:G:H5'   | 2.01                     | 0.59              |
| 25:DC:136:VAL:CA  | 25:DC:165:ALA:HA   | 2.33                     | 0.59              |
| 25:DC:138:SER:HA  | 25:DC:162:GLN:HG3  | 1.85                     | 0.59              |
| 28:DF:53:ALA:HB1  | 28:DF:64:PRO:HG2   | 1.84                     | 0.59              |
| 29:DG:148:ARG:HA  | 29:DG:161:VAL:HG13 | 1.85                     | 0.59              |
| 38:DQ:54:ARG:O    | 38:DQ:58:GLN:HG2   | 2.02                     | 0.59              |
| 40:DS:25:ARG:HD2  | 40:DS:26:GLY:H     | 1.65                     | 0.59              |
| 43:DW:44:PHE:HB3  | 43:DW:77:LYS:CB    | 2.32                     | 0.59              |
| 45:DY:6:ILE:HG13  | 45:DY:35:VAL:H     | 1.66                     | 0.59              |
| 1:AA:214:C:H2'    | 1:AA:215:C:C6      | 2.38                     | 0.59              |
| 1:AA:1042:A:H2'   | 1:AA:1043:G:O4'    | 2.02                     | 0.59              |
| 2:AC:13:ILE:HG22  | 2:AC:14:VAL:HG13   | 1.83                     | 0.59              |
| 4:AE:37:VAL:HG11  | 4:AE:113:VAL:HG12  | 1.83                     | 0.59              |
| 22:BA:21:G:O2'    | 22:BA:22:U:H5'     | 2.02                     | 0.59              |
| 22:BA:24:G:N7     | 22:BA:56:G:H2'     | 2.17                     | 0.59              |
| 22:BA:29:A:H3'    | 22:BA:30:C:H6      | 1.67                     | 0.59              |
| 23:BB:79:C:O2'    | 23:BB:346:A:H1'    | 2.02                     | 0.59              |
| 23:BB:359:G:O2'   | 23:BB:360:U:H5'    | 2.02                     | 0.59              |
| 23:BB:445:C:H5'   | 27:BE:47:LYS:NZ    | 2.17                     | 0.59              |
| 23:BB:1162:G:H4'  | 39:BR:23:GLU:HG2   | 1.83                     | 0.59              |
| 23:BB:1412:U:H2'  | 23:BB:1413:A:C8    | 2.38                     | 0.59              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:BB:1444:G:H2'   | 23:BB:1445:G:H8   | 1.67                     | 0.59              |
| 23:BB:1676:A:H2'   | 23:BB:1677:A:O4'  | 2.02                     | 0.59              |
| 23:BB:2077:A:H2'   | 23:BB:2078:C:C6   | 2.36                     | 0.59              |
| 23:BB:2893:A:H5''  | 23:BB:2894:G:H5'  | 1.85                     | 0.59              |
| 26:BD:4:LEU:O      | 26:BD:5:VAL:HG13  | 2.02                     | 0.59              |
| 28:BF:115:GLY:HA3  | 28:BF:177:ARG:HB2 | 1.84                     | 0.59              |
| 29:BG:131:VAL:HG13 | 29:BG:133:LYS:HE2 | 1.85                     | 0.59              |
| 31:BJ:55:ILE:HA    | 31:BJ:122:LEU:O   | 2.02                     | 0.59              |
| 33:BL:13:LYS:O     | 33:BL:14:LYS:HB2  | 2.01                     | 0.59              |
| 35:BN:45:ARG:HB2   | 35:BN:49:GLU:OE2  | 2.03                     | 0.59              |
| 37:BP:77:SER:H     | 37:BP:78:PRO:HD2  | 1.68                     | 0.59              |
| 38:BQ:88:GLU:HA    | 39:BR:53:PHE:CZ   | 2.36                     | 0.59              |
| 40:BS:52:GLU:HA    | 40:BS:55:ILE:HG22 | 1.85                     | 0.59              |
| 1:CA:1030:U:H5''   | 1:CA:1031:C:H5    | 1.68                     | 0.59              |
| 1:CA:1107:C:H4'    | 2:CC:172:VAL:HG23 | 1.83                     | 0.59              |
| 1:CA:1251:A:O2'    | 1:CA:1252:A:H5'   | 2.02                     | 0.59              |
| 1:CA:1308:U:H2'    | 1:CA:1309:G:C8    | 2.38                     | 0.59              |
| 10:CK:53:GLY:HA2   | 10:CK:56:LYS:HE3  | 1.84                     | 0.59              |
| 10:CK:82:GLU:HB3   | 10:CK:108:ASN:ND2 | 2.16                     | 0.59              |
| 13:CN:96:LYS:HG2   | 13:CN:97:LYS:N    | 2.14                     | 0.59              |
| 15:CP:4:ILE:HD13   | 15:CP:57:ILE:HG12 | 1.85                     | 0.59              |
| 16:CQ:16:MET:CB    | 16:CQ:19:SER:HB2  | 2.33                     | 0.59              |
| 16:CQ:23:ALA:C     | 16:CQ:24:ILE:HD12 | 2.27                     | 0.59              |
| 17:CR:55:ALA:O     | 17:CR:59:LYS:HG3  | 2.03                     | 0.59              |
| 18:CS:38:THR:HG22  | 18:CS:39:ILE:H    | 1.66                     | 0.59              |
| 20:CB:116:LEU:O    | 20:CB:119:GLN:HB2 | 2.02                     | 0.59              |
| 23:DB:659:G:H4'    | 27:DE:95:LYS:HD3  | 1.85                     | 0.59              |
| 23:DB:1013:C:H2'   | 23:DB:1014:A:H8   | 1.66                     | 0.59              |
| 23:DB:1447:C:H2'   | 23:DB:1448:G:C8   | 2.37                     | 0.59              |
| 23:DB:1550:C:H2'   | 23:DB:1551:A:H8   | 1.67                     | 0.59              |
| 23:DB:1742:U:H2'   | 23:DB:1743:G:C8   | 2.38                     | 0.59              |
| 23:DB:2220:U:H2'   | 23:DB:2221:G:H8   | 1.68                     | 0.59              |
| 23:DB:2324:U:H3'   | 23:DB:2325:G:C5'  | 2.32                     | 0.59              |
| 23:DB:2852:G:H2'   | 23:DB:2853:C:H6   | 1.67                     | 0.59              |
| 23:DB:2899:A:H2'   | 23:DB:2900:A:C8   | 2.37                     | 0.59              |
| 24:DV:9:ARG:HH21   | 24:DV:20:LEU:HD11 | 1.68                     | 0.59              |
| 26:DD:31:ALA:CB    | 26:DD:95:SER:HB2  | 2.32                     | 0.59              |
| 26:DD:52:THR:OG1   | 26:DD:75:ALA:HB1  | 2.02                     | 0.59              |
| 27:DE:116:ASP:CB   | 27:DE:185:LYS:HA  | 2.30                     | 0.59              |
| 28:DF:135:ILE:O    | 28:DF:137:PHE:N   | 2.36                     | 0.59              |
| 31:DJ:15:TRP:CD2   | 31:DJ:138:GLN:HB2 | 2.38                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:DM:131:VAL:HG22 | 34:DM:133:LYS:H    | 1.68                     | 0.59              |
| 36:DO:74:VAL:O     | 36:DO:78:VAL:HG23  | 2.02                     | 0.59              |
| 37:DP:90:ALA:HB3   | 37:DP:112:ARG:H    | 1.67                     | 0.59              |
| 41:DT:24:MET:HE2   | 41:DT:30:ILE:HA    | 1.85                     | 0.59              |
| 1:AA:766:A:H2      | 1:AA:1525:G:N3     | 1.99                     | 0.59              |
| 1:AA:796:C:H5'     | 10:AK:128:VAL:HG13 | 1.84                     | 0.59              |
| 1:AA:1130:A:H2'    | 1:AA:1131:G:H8     | 1.68                     | 0.59              |
| 5:AF:18:VAL:O      | 5:AF:22:ILE:HG13   | 2.02                     | 0.59              |
| 16:AQ:4:ILE:H      | 16:AQ:4:ILE:HD12   | 1.67                     | 0.59              |
| 23:BB:209:C:H2'    | 23:BB:210:C:H6     | 1.67                     | 0.59              |
| 23:BB:222:A:N1     | 23:BB:233:A:H5''   | 2.17                     | 0.59              |
| 23:BB:1312:U:OP2   | 41:BT:66:LYS:HG2   | 2.02                     | 0.59              |
| 23:BB:1470:A:H3'   | 23:BB:1471:G:H8    | 1.67                     | 0.59              |
| 25:BC:163:ILE:HG22 | 25:BC:164:VAL:N    | 2.16                     | 0.59              |
| 27:BE:132:LYS:HD3  | 27:BE:133:LEU:CD2  | 2.32                     | 0.59              |
| 27:BE:193:VAL:HG12 | 27:BE:194:LYS:HD2  | 1.84                     | 0.59              |
| 29:BG:18:ILE:HD13  | 29:BG:18:ILE:H     | 1.66                     | 0.59              |
| 29:BG:102:ILE:HG23 | 29:BG:104:LEU:HD11 | 1.83                     | 0.59              |
| 29:BG:119:GLY:C    | 29:BG:120:ILE:HD12 | 2.27                     | 0.59              |
| 31:BJ:128:ASN:CG   | 31:BJ:129:GLU:H    | 2.08                     | 0.59              |
| 34:BM:73:ILE:HG12  | 34:BM:90:GLU:OE2   | 2.03                     | 0.59              |
| 37:BP:5:LYS:C      | 37:BP:7:LEU:H      | 2.09                     | 0.59              |
| 37:BP:92:ARG:CZ    | 37:BP:110:LYS:HB3  | 2.33                     | 0.59              |
| 38:BQ:102:LYS:HD2  | 38:BQ:102:LYS:N    | 2.18                     | 0.59              |
| 48:B1:42:VAL:HB    | 48:B1:43:ARG:HH21  | 1.67                     | 0.59              |
| 52:BI:14:ALA:HA    | 52:BI:45:THR:HG21  | 1.83                     | 0.59              |
| 1:CA:121:U:OP1     | 1:CA:121:U:H3'     | 2.03                     | 0.59              |
| 3:CD:2:ARG:HH11    | 3:CD:114:ARG:HD3   | 1.65                     | 0.59              |
| 5:CF:92:THR:HG22   | 5:CF:93:LYS:N      | 2.18                     | 0.59              |
| 23:DB:587:C:H5'    | 27:DE:85:PHE:CE1   | 2.37                     | 0.59              |
| 23:DB:634:C:H2'    | 23:DB:635:C:C6     | 2.38                     | 0.59              |
| 23:DB:1262:A:C2    | 47:D0:6:LYS:HD2    | 2.36                     | 0.59              |
| 23:DB:1825:U:H5'   | 25:DC:244:VAL:HG21 | 1.83                     | 0.59              |
| 23:DB:2758:A:H2'   | 23:DB:2759:G:H5'   | 1.85                     | 0.59              |
| 28:DF:26:GLN:HG2   | 28:DF:26:GLN:O     | 2.03                     | 0.59              |
| 30:DH:103:VAL:HG13 | 30:DH:108:VAL:HB   | 1.84                     | 0.59              |
| 30:DH:129:GLU:HA   | 30:DH:143:ILE:HA   | 1.85                     | 0.59              |
| 31:DJ:36:LEU:HD13  | 31:DJ:54:ILE:HD12  | 1.83                     | 0.59              |
| 36:DO:15:ARG:HH22  | 43:DW:76:ARG:HG2   | 1.68                     | 0.59              |
| 41:DT:15:HIS:O     | 41:DT:16:VAL:HB    | 2.01                     | 0.59              |
| 1:AA:390:U:H2'     | 1:AA:391:G:H8      | 1.62                     | 0.59              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:522:C:H41     | 11:AL:49:ARG:HH22  | 1.49                     | 0.59              |
| 1:AA:716:A:N3      | 10:AK:119:GLY:HA2  | 2.17                     | 0.59              |
| 2:AC:21:TRP:CB     | 2:AC:58:ARG:HB2    | 2.33                     | 0.59              |
| 8:AI:35:GLU:HA     | 8:AI:39:GLY:CA     | 2.33                     | 0.59              |
| 10:AK:81:LEU:HD22  | 10:AK:104:PHE:HB3  | 1.84                     | 0.59              |
| 19:AT:54:GLN:N     | 19:AT:55:PRO:HD2   | 2.17                     | 0.59              |
| 20:AB:46:VAL:HA    | 20:AB:49:PHE:HD2   | 1.68                     | 0.59              |
| 20:AB:206:ILE:HD13 | 20:AB:206:ILE:O    | 2.02                     | 0.59              |
| 23:BB:419:U:H2'    | 23:BB:420:C:H6     | 1.67                     | 0.59              |
| 23:BB:441:U:H2'    | 23:BB:442:G:H8     | 1.67                     | 0.59              |
| 23:BB:483:A:H4'    | 42:BU:45:GLN:HA    | 1.83                     | 0.59              |
| 23:BB:1007:C:H5''  | 31:BJ:37:ARG:NH2   | 2.18                     | 0.59              |
| 23:BB:1241:A:H2'   | 23:BB:1242:U:C5'   | 2.32                     | 0.59              |
| 23:BB:2467:C:O4'   | 34:BM:118:LYS:HG2  | 2.02                     | 0.59              |
| 23:BB:2617:U:H2'   | 23:BB:2618:G:H5'   | 1.85                     | 0.59              |
| 24:BV:40:ILE:HD13  | 24:BV:40:ILE:N     | 2.18                     | 0.59              |
| 25:BC:30:ALA:N     | 25:BC:31:PRO:CD    | 2.66                     | 0.59              |
| 28:BF:70:ARG:HA    | 28:BF:80:GLN:HG3   | 1.83                     | 0.59              |
| 30:BH:4:ILE:C      | 30:BH:37:VAL:HG12  | 2.27                     | 0.59              |
| 33:BL:131:ALA:HB1  | 33:BL:135:ILE:HD12 | 1.85                     | 0.59              |
| 34:BM:86:LYS:HD2   | 34:BM:86:LYS:H     | 1.68                     | 0.59              |
| 41:BT:32:LEU:C     | 41:BT:34:VAL:H     | 2.11                     | 0.59              |
| 47:B0:2:VAL:HG22   | 47:B0:3:GLN:H      | 1.67                     | 0.59              |
| 47:B0:35:GLU:CD    | 47:B0:43:THR:HG22  | 2.28                     | 0.59              |
| 1:CA:1031:C:H4'    | 1:CA:1032:G:H5''   | 1.84                     | 0.59              |
| 1:CA:1326:U:O2'    | 1:CA:1327:C:H5'    | 2.02                     | 0.59              |
| 2:CC:65:VAL:HG21   | 2:CC:90:VAL:HG11   | 1.83                     | 0.59              |
| 21:CU:24:LYS:HD2   | 21:CU:25:ALA:N     | 2.11                     | 0.59              |
| 23:DB:79:C:O2'     | 23:DB:346:A:H1'    | 2.03                     | 0.59              |
| 23:DB:213:A:O2'    | 23:DB:214:G:H5'    | 2.03                     | 0.59              |
| 23:DB:299:A:N6     | 23:DB:322:A:O2'    | 2.33                     | 0.59              |
| 23:DB:324:A:OP2    | 27:DE:164:LEU:HB2  | 2.02                     | 0.59              |
| 23:DB:1099:G:O4'   | 52:DI:3:LYS:O      | 2.20                     | 0.59              |
| 23:DB:1111:A:H4'   | 29:DG:1:SER:O      | 2.03                     | 0.59              |
| 23:DB:1210:G:H4'   | 23:DB:1211:C:OP2   | 2.02                     | 0.59              |
| 23:DB:1412:U:H2'   | 23:DB:1413:A:C8    | 2.38                     | 0.59              |
| 23:DB:2859:G:H2'   | 23:DB:2860:A:C8    | 2.36                     | 0.59              |
| 24:DV:9:ARG:HG2    | 24:DV:41:GLU:CG    | 2.32                     | 0.59              |
| 25:DC:163:ILE:HG12 | 25:DC:173:LEU:CD2  | 2.33                     | 0.59              |
| 25:DC:261:ARG:HG2  | 25:DC:261:ARG:HH11 | 1.66                     | 0.59              |
| 26:DD:22:ILE:O     | 26:DD:22:ILE:HG13  | 2.01                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:DD:77:ARG:HB2   | 26:DD:77:ARG:HH11  | 1.67                     | 0.59              |
| 28:DF:133:GLU:H    | 28:DF:150:GLY:HA2  | 1.66                     | 0.59              |
| 30:DH:89:LYS:HA    | 30:DH:123:ARG:O    | 2.03                     | 0.59              |
| 33:DL:2:ARG:HG3    | 33:DL:2:ARG:NH1    | 2.18                     | 0.59              |
| 33:DL:64:PHE:HD2   | 50:D3:11:LYS:HB3   | 1.68                     | 0.59              |
| 33:DL:85:VAL:HG13  | 33:DL:86:GLU:N     | 2.11                     | 0.59              |
| 34:DM:40:ARG:HA    | 34:DM:92:TRP:NE1   | 2.17                     | 0.59              |
| 35:DN:41:ALA:HB1   | 35:DN:113:ILE:CD1  | 2.32                     | 0.59              |
| 44:DX:25:GLN:O     | 44:DX:29:ARG:HG3   | 2.02                     | 0.59              |
| 1:AA:121:U:OP1     | 1:AA:121:U:H3'     | 2.03                     | 0.59              |
| 1:AA:801:U:H2'     | 1:AA:802:A:H8      | 1.67                     | 0.59              |
| 4:AE:110:MET:O     | 4:AE:113:VAL:HG22  | 2.03                     | 0.59              |
| 6:AG:117:LEU:HD22  | 6:AG:120:ALA:HB3   | 1.84                     | 0.59              |
| 12:AM:64:VAL:HG12  | 12:AM:65:GLU:N     | 2.18                     | 0.59              |
| 23:BB:156:A:H2'    | 23:BB:157:C:H6     | 1.67                     | 0.59              |
| 23:BB:296:U:H2'    | 23:BB:297:G:H8     | 1.67                     | 0.59              |
| 23:BB:355:U:H2'    | 23:BB:356:G:H8     | 1.68                     | 0.59              |
| 23:BB:544:C:H2'    | 23:BB:545:U:C2     | 2.38                     | 0.59              |
| 23:BB:1429:G:H2'   | 23:BB:1430:G:C8    | 2.37                     | 0.59              |
| 23:BB:2097:A:H2'   | 23:BB:2098:U:C6    | 2.38                     | 0.59              |
| 23:BB:2328:A:H2'   | 23:BB:2329:U:H6    | 1.67                     | 0.59              |
| 30:BH:62:LEU:O     | 30:BH:66:ASN:HB3   | 2.03                     | 0.59              |
| 35:BN:24:MET:O     | 35:BN:27:SER:HB3   | 2.03                     | 0.59              |
| 35:BN:107:ASN:HD21 | 40:BS:40:ASN:CG    | 2.11                     | 0.59              |
| 39:BR:47:VAL:HG13  | 39:BR:49:ILE:N     | 2.13                     | 0.59              |
| 52:BI:32:VAL:HG22  | 52:BI:60:VAL:HG21  | 1.85                     | 0.59              |
| 1:CA:501:C:H1'     | 1:CA:549:C:H1'     | 1.85                     | 0.59              |
| 1:CA:812:G:O2'     | 1:CA:813:U:H6      | 1.85                     | 0.59              |
| 1:CA:939:G:H5''    | 6:CG:101:ARG:NH2   | 2.17                     | 0.59              |
| 1:CA:993:G:H2'     | 1:CA:995:C:H41     | 1.66                     | 0.59              |
| 1:CA:1238:A:C2     | 1:CA:1241:G:H1'    | 2.38                     | 0.59              |
| 13:CN:86:ALA:HB1   | 13:CN:91:GLU:HB2   | 1.84                     | 0.59              |
| 23:DB:95:A:O2'     | 44:DX:43:LEU:HD21  | 2.03                     | 0.59              |
| 23:DB:635:C:H3'    | 33:DL:126:ARG:NH2  | 2.18                     | 0.59              |
| 23:DB:850:U:O2'    | 45:DY:22:THR:HG22  | 2.03                     | 0.59              |
| 23:DB:2181:U:O5'   | 23:DB:2181:U:H6    | 1.86                     | 0.59              |
| 23:DB:2369:A:O2'   | 23:DB:2370:G:H5'   | 2.03                     | 0.59              |
| 25:DC:140:VAL:HG11 | 25:DC:163:ILE:HD11 | 1.84                     | 0.59              |
| 25:DC:171:VAL:HB   | 25:DC:182:LYS:CB   | 2.26                     | 0.59              |
| 32:DK:99:ILE:CD1   | 32:DK:115:ILE:HG13 | 2.32                     | 0.59              |
| 33:DL:109:LYS:CG   | 33:DL:126:ARG:HD3  | 2.33                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:DR:6:GLN:OE1   | 39:DR:38:VAL:HG22 | 2.02                     | 0.59              |
| 40:DS:27:LYS:HG3  | 40:DS:70:LYS:HD3  | 1.85                     | 0.59              |
| 1:AA:202:G:H2'    | 1:AA:203:G:C8     | 2.37                     | 0.59              |
| 1:AA:300:A:H2'    | 1:AA:301:G:O4'    | 2.03                     | 0.59              |
| 1:AA:1348:U:OP1   | 8:AI:111:GLU:HB2  | 2.02                     | 0.59              |
| 10:AK:84:MET:HE2  | 10:AK:110:THR:OG1 | 2.02                     | 0.59              |
| 16:AQ:26:ARG:HH21 | 16:AQ:39:ARG:NH1  | 2.00                     | 0.59              |
| 23:BB:170:U:H2'   | 23:BB:171:U:C6    | 2.37                     | 0.59              |
| 23:BB:1076:C:H4'  | 52:BI:94:LYS:CE   | 2.33                     | 0.59              |
| 23:BB:1579:A:H2'  | 23:BB:1580:A:C8   | 2.38                     | 0.59              |
| 23:BB:2188:U:H2'  | 23:BB:2189:U:C6   | 2.37                     | 0.59              |
| 23:BB:2261:C:OP2  | 43:BW:13:ARG:HB2  | 2.03                     | 0.59              |
| 23:BB:2491:U:H5'' | 23:BB:2570:G:C5'  | 2.33                     | 0.59              |
| 23:BB:2789:C:H3'  | 23:BB:2893:A:H62  | 1.66                     | 0.59              |
| 28:BF:15:LEU:HD13 | 28:BF:28:PRO:HG2  | 1.83                     | 0.59              |
| 29:BG:17:LYS:HB3  | 29:BG:24:THR:HG22 | 1.85                     | 0.59              |
| 33:BL:40:SER:C    | 33:BL:41:ARG:HE   | 2.10                     | 0.59              |
| 35:BN:38:LEU:HB2  | 35:BN:109:PRO:CB  | 2.33                     | 0.59              |
| 37:BP:59:THR:HA   | 37:BP:76:HIS:HA   | 1.84                     | 0.59              |
| 39:BR:90:ARG:HH11 | 39:BR:91:GLN:N    | 2.01                     | 0.59              |
| 40:BS:66:ILE:HD12 | 40:BS:66:ILE:N    | 2.18                     | 0.59              |
| 42:BU:13:LEU:HD12 | 42:BU:69:VAL:HA   | 1.84                     | 0.59              |
| 42:BU:73:ASN:HB2  | 42:BU:96:LYS:NZ   | 2.18                     | 0.59              |
| 44:BX:35:GLY:CA   | 44:BX:40:SER:HA   | 2.32                     | 0.59              |
| 46:BZ:15:SER:O    | 46:BZ:21:VAL:HB   | 2.02                     | 0.59              |
| 52:BI:18:ASN:N    | 52:BI:19:PRO:HD2  | 2.17                     | 0.59              |
| 52:BI:77:VAL:HA   | 52:BI:80:LYS:CE   | 2.33                     | 0.59              |
| 1:CA:131:A:H2'    | 1:CA:132:C:H6     | 1.68                     | 0.59              |
| 1:CA:529:G:O6     | 11:CL:45:ASN:HA   | 2.03                     | 0.59              |
| 1:CA:1019:A:H2'   | 1:CA:1020:G:C8    | 2.38                     | 0.59              |
| 4:CE:95:MET:HG3   | 4:CE:124:ALA:HB2  | 1.83                     | 0.59              |
| 7:CH:54:THR:HG23  | 7:CH:55:LYS:HG2   | 1.83                     | 0.59              |
| 8:CI:38:PHE:O     | 8:CI:44:ARG:HD2   | 2.03                     | 0.59              |
| 14:CO:28:VAL:HG11 | 14:CO:80:LEU:HD21 | 1.85                     | 0.59              |
| 23:DB:794:A:H2'   | 23:DB:795:C:H6    | 1.67                     | 0.59              |
| 23:DB:873:C:H2'   | 23:DB:874:G:H8    | 1.68                     | 0.59              |
| 23:DB:1442:U:H2'  | 23:DB:1443:U:H6   | 1.68                     | 0.59              |
| 23:DB:1470:A:H3'  | 23:DB:1471:G:H8   | 1.66                     | 0.59              |
| 28:DF:65:LEU:CD2  | 28:DF:87:LYS:HD2  | 2.33                     | 0.59              |
| 31:DJ:21:THR:HG22 | 31:DJ:58:ASN:OD1  | 2.03                     | 0.59              |
| 41:DT:66:LYS:HB3  | 41:DT:66:LYS:HZ2  | 1.67                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 42:DU:31:GLY:O    | 42:DU:32:LYS:HD3  | 2.03                     | 0.59              |
| 49:D2:13:ASN:HA   | 49:D2:16:HIS:O    | 2.02                     | 0.59              |
| 1:AA:403:C:O2'    | 1:AA:404:G:H5'    | 2.02                     | 0.58              |
| 1:AA:1448:C:H2'   | 1:AA:1449:C:C6    | 2.38                     | 0.58              |
| 3:AD:144:ILE:CD1  | 3:AD:154:VAL:HG21 | 2.33                     | 0.58              |
| 12:AM:2:ARG:HB3   | 12:AM:6:ILE:O     | 2.03                     | 0.58              |
| 19:AT:53:MET:O    | 19:AT:57:VAL:HG23 | 2.02                     | 0.58              |
| 23:BB:131:A:H2'   | 23:BB:132:G:C8    | 2.38                     | 0.58              |
| 23:BB:1387:A:H5'  | 23:BB:1469:A:H1'  | 1.84                     | 0.58              |
| 23:BB:1454:C:H5'  | 35:BN:63:ARG:NH2  | 2.07                     | 0.58              |
| 23:BB:1484:U:H2'  | 23:BB:1485:U:C6   | 2.37                     | 0.58              |
| 23:BB:1484:U:H2'  | 23:BB:1485:U:H6   | 1.68                     | 0.58              |
| 23:BB:1652:A:H62  | 35:BN:11:ASN:ND2  | 2.01                     | 0.58              |
| 23:BB:2789:C:H2'  | 23:BB:2893:A:N7   | 2.17                     | 0.58              |
| 30:BH:37:VAL:O    | 30:BH:38:PRO:C    | 2.46                     | 0.58              |
| 31:BJ:20:ALA:HB1  | 31:BJ:59:ALA:CA   | 2.33                     | 0.58              |
| 32:BK:60:ALA:HA   | 32:BK:87:LEU:HG   | 1.84                     | 0.58              |
| 32:BK:104:THR:O   | 32:BK:107:LEU:HB3 | 2.03                     | 0.58              |
| 34:BM:8:LYS:HB2   | 34:BM:12:MET:HE3  | 1.84                     | 0.58              |
| 38:BQ:97:ILE:HA   | 38:BQ:100:PHE:CZ  | 2.38                     | 0.58              |
| 39:BR:7:SER:C     | 39:BR:22:LEU:HD11 | 2.27                     | 0.58              |
| 40:BS:7:HIS:CD2   | 40:BS:10:ALA:HB2  | 2.38                     | 0.58              |
| 41:BT:36:LYS:HD3  | 41:BT:36:LYS:O    | 2.01                     | 0.58              |
| 50:B3:23:HIS:H    | 50:B3:23:HIS:HD2  | 1.50                     | 0.58              |
| 1:CA:34:C:H2'     | 1:CA:35:G:H8      | 1.68                     | 0.58              |
| 1:CA:476:U:H2'    | 1:CA:477:C:C6     | 2.38                     | 0.58              |
| 4:CE:24:VAL:HG23  | 4:CE:26:GLY:H     | 1.67                     | 0.58              |
| 4:CE:61:LYS:O     | 4:CE:64:GLU:HB3   | 2.03                     | 0.58              |
| 22:DA:66:A:HO2'   | 22:DA:67:G:H8     | 1.51                     | 0.58              |
| 23:DB:136:G:N1    | 41:DT:3:ARG:NH1   | 2.51                     | 0.58              |
| 23:DB:672:C:O2'   | 23:DB:673:C:H5'   | 2.03                     | 0.58              |
| 23:DB:1059:G:H4'  | 52:DI:116:MET:HE2 | 1.83                     | 0.58              |
| 26:DD:110:THR:HB  | 26:DD:202:ILE:HB  | 1.84                     | 0.58              |
| 27:DE:152:GLU:O   | 27:DE:153:LEU:HB2 | 2.02                     | 0.58              |
| 30:DH:98:ASP:HA   | 30:DH:101:ASP:OD1 | 2.03                     | 0.58              |
| 31:DJ:23:LYS:C    | 31:DJ:25:LEU:HD13 | 2.28                     | 0.58              |
| 32:DK:24:VAL:HG13 | 32:DK:33:ALA:HB2  | 1.85                     | 0.58              |
| 33:DL:118:THR:OG1 | 33:DL:138:ALA:HB2 | 2.02                     | 0.58              |
| 33:DL:123:ARG:HB3 | 33:DL:141:LYS:HB3 | 1.83                     | 0.58              |
| 36:DO:93:ASP:HB2  | 36:DO:117:PHE:CE2 | 2.38                     | 0.58              |
| 37:DP:25:VAL:CG1  | 37:DP:87:ARG:HA   | 2.29                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 37:DP:65:ASN:H     | 37:DP:71:ARG:HA   | 1.68                     | 0.58              |
| 38:DQ:20:ALA:HA    | 38:DQ:23:TYR:CE2  | 2.37                     | 0.58              |
| 38:DQ:87:VAL:HB    | 39:DR:54:VAL:HG11 | 1.85                     | 0.58              |
| 42:DU:66:VAL:HG22  | 42:DU:67:SER:N    | 2.08                     | 0.58              |
| 42:DU:98:ASN:O     | 42:DU:99:SER:HB2  | 2.01                     | 0.58              |
| 43:DW:65:LYS:HB2   | 43:DW:65:LYS:NZ   | 2.18                     | 0.58              |
| 1:AA:241:G:O2'     | 1:AA:242:G:H5'    | 2.03                     | 0.58              |
| 1:AA:408:A:H5'     | 3:AD:21:LYS:HE2   | 1.84                     | 0.58              |
| 1:AA:687:A:C2      | 1:AA:704:A:C5     | 2.91                     | 0.58              |
| 1:AA:1011:C:H2'    | 1:AA:1012:A:C8    | 2.38                     | 0.58              |
| 1:AA:1237:C:H3'    | 1:AA:1238:A:H5'   | 1.85                     | 0.58              |
| 2:AC:141:MET:HA    | 2:AC:141:MET:HE3  | 1.83                     | 0.58              |
| 5:AF:42:TRP:HB2    | 5:AF:59:TYR:HB2   | 1.84                     | 0.58              |
| 10:AK:113:THR:CG2  | 21:AU:28:LEU:HD21 | 2.33                     | 0.58              |
| 12:AM:72:ILE:O     | 12:AM:76:ILE:HG13 | 2.03                     | 0.58              |
| 15:AP:46:LYS:H     | 15:AP:46:LYS:HE2  | 1.65                     | 0.58              |
| 20:AB:60:ALA:HB3   | 20:AB:223:GLY:HA3 | 1.83                     | 0.58              |
| 23:BB:156:A:H2'    | 23:BB:157:C:C6    | 2.38                     | 0.58              |
| 23:BB:686:U:O4     | 49:B2:12:ARG:HG3  | 2.02                     | 0.58              |
| 23:BB:1945:G:H2'   | 23:BB:1946:U:C6   | 2.37                     | 0.58              |
| 23:BB:2369:A:O2'   | 23:BB:2370:G:H5'  | 2.03                     | 0.58              |
| 23:BB:2386:A:H2'   | 23:BB:2387:U:C6   | 2.38                     | 0.58              |
| 23:BB:2480:C:O2'   | 23:BB:2481:G:H5'  | 2.03                     | 0.58              |
| 24:BV:84:PRO:HG3   | 34:BM:127:LYS:HE2 | 1.85                     | 0.58              |
| 30:BH:94:ILE:HG23  | 30:BH:99:ILE:HD11 | 1.84                     | 0.58              |
| 31:BJ:18:VAL:HG22  | 31:BJ:55:ILE:O    | 2.02                     | 0.58              |
| 31:BJ:77:HIS:CD2   | 31:BJ:84:ILE:HB   | 2.38                     | 0.58              |
| 34:BM:38:ARG:HH11  | 34:BM:38:ARG:CB   | 2.10                     | 0.58              |
| 37:BP:28:LYS:HG2   | 37:BP:44:GLY:O    | 2.03                     | 0.58              |
| 37:BP:31:VAL:HG12  | 37:BP:33:GLU:H    | 1.68                     | 0.58              |
| 37:BP:59:THR:HG23  | 37:BP:76:HIS:NE2  | 2.18                     | 0.58              |
| 42:BU:70:ALA:HB3   | 42:BU:77:GLY:O    | 2.03                     | 0.58              |
| 52:BI:105:LEU:HD11 | 52:BI:139:VAL:CG1 | 2.33                     | 0.58              |
| 1:CA:413:G:H4'     | 1:CA:414:A:H5''   | 1.85                     | 0.58              |
| 1:CA:1119:C:H2'    | 1:CA:1120:C:C6    | 2.37                     | 0.58              |
| 3:CD:30:LYS:HB2    | 3:CD:30:LYS:NZ    | 2.18                     | 0.58              |
| 3:CD:71:PHE:HE2    | 3:CD:89:LEU:HD11  | 1.68                     | 0.58              |
| 12:CM:89:ARG:HB3   | 12:CM:96:VAL:HG22 | 1.84                     | 0.58              |
| 23:DB:28:A:O2'     | 23:DB:29:U:H5'    | 2.03                     | 0.58              |
| 23:DB:1857:G:H1'   | 23:DB:1885:A:N6   | 2.16                     | 0.58              |
| 23:DB:2022:U:O2'   | 23:DB:2617:U:H5'  | 2.03                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:2836:U:H2'   | 23:DB:2837:A:C8    | 2.39                     | 0.58              |
| 23:DB:2887:A:N9    | 47:D0:27:LEU:HD21  | 2.18                     | 0.58              |
| 25:DC:87:SER:N     | 25:DC:155:ARG:HH12 | 2.01                     | 0.58              |
| 28:DF:107:VAL:HG11 | 28:DF:175:PRO:HG3  | 1.85                     | 0.58              |
| 29:DG:41:GLU:HG2   | 29:DG:54:ARG:HH21  | 1.68                     | 0.58              |
| 31:DJ:59:ALA:C     | 31:DJ:61:LYS:H     | 2.12                     | 0.58              |
| 34:DM:41:LEU:HG    | 34:DM:46:ILE:HD11  | 1.85                     | 0.58              |
| 36:DO:9:ARG:C      | 36:DO:11:ALA:H     | 2.11                     | 0.58              |
| 37:DP:7:LEU:O      | 37:DP:11:GLN:HG2   | 2.03                     | 0.58              |
| 38:DQ:39:ILE:HG13  | 38:DQ:40:LYS:N     | 2.17                     | 0.58              |
| 50:D3:14:LYS:HA    | 50:D3:63:TYR:CE2   | 2.38                     | 0.58              |
| 1:AA:203:G:N2      | 1:AA:205:A:H61     | 2.01                     | 0.58              |
| 1:AA:950:U:H2'     | 1:AA:951:G:H8      | 1.68                     | 0.58              |
| 1:AA:1246:A:H2'    | 1:AA:1247:U:C6     | 2.38                     | 0.58              |
| 13:AN:71:GLY:O     | 13:AN:79:SER:HA    | 2.04                     | 0.58              |
| 18:AS:4:LEU:HD13   | 18:AS:8:PRO:HA     | 1.84                     | 0.58              |
| 20:AB:67:LEU:HD13  | 20:AB:67:LEU:N     | 2.18                     | 0.58              |
| 23:BB:37:C:H2'     | 27:BE:46:GLN:OE1   | 2.03                     | 0.58              |
| 23:BB:877:A:N1     | 23:BB:899:A:H2'    | 2.17                     | 0.58              |
| 23:BB:1447:C:H2'   | 23:BB:1448:G:C8    | 2.37                     | 0.58              |
| 23:BB:1552:A:C2'   | 23:BB:1553:A:H5'   | 2.33                     | 0.58              |
| 23:BB:2836:U:H2'   | 23:BB:2837:A:C8    | 2.39                     | 0.58              |
| 25:BC:32:LEU:HA    | 25:BC:81:GLU:OE1   | 2.04                     | 0.58              |
| 27:BE:3:LEU:CB     | 27:BE:12:LEU:HD22  | 2.33                     | 0.58              |
| 28:BF:132:ARG:NE   | 28:BF:147:ARG:HE   | 2.00                     | 0.58              |
| 30:BH:35:LYS:O     | 30:BH:37:VAL:HG13  | 2.03                     | 0.58              |
| 30:BH:73:ASN:ND2   | 30:BH:73:ASN:N     | 2.52                     | 0.58              |
| 31:BJ:75:TYR:HA    | 31:BJ:86:GLN:O     | 2.04                     | 0.58              |
| 32:BK:11:ALA:HB3   | 32:BK:85:VAL:HG23  | 1.85                     | 0.58              |
| 34:BM:35:ALA:HB3   | 34:BM:97:GLN:C     | 2.28                     | 0.58              |
| 42:BU:46:LYS:HE2   | 42:BU:54:PRO:O     | 2.03                     | 0.58              |
| 51:B4:16:ILE:HD12  | 51:B4:16:ILE:N     | 2.17                     | 0.58              |
| 1:CA:300:A:H2'     | 1:CA:301:G:O4'     | 2.03                     | 0.58              |
| 1:CA:1163:A:H2'    | 1:CA:1164:G:H8     | 1.67                     | 0.58              |
| 4:CE:11:GLN:OE1    | 4:CE:116:VAL:HA    | 2.03                     | 0.58              |
| 4:CE:113:VAL:HG23  | 4:CE:114:LEU:N     | 2.18                     | 0.58              |
| 8:CI:41:GLU:H      | 8:CI:44:ARG:HD3    | 1.68                     | 0.58              |
| 9:CJ:38:GLY:O      | 9:CJ:74:VAL:HA     | 2.03                     | 0.58              |
| 9:CJ:85:ASP:HA     | 9:CJ:89:ARG:HB2    | 1.85                     | 0.58              |
| 10:CK:73:VAL:O     | 10:CK:76:TYR:HB2   | 2.04                     | 0.58              |
| 14:CO:20:ASP:OD2   | 14:CO:23:SER:HB2   | 2.04                     | 0.58              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:38:C:H4'     | 36:DO:100:HIS:NE2  | 2.18                     | 0.58              |
| 23:DB:230:G:H2'    | 23:DB:231:A:H8     | 1.67                     | 0.58              |
| 23:DB:307:G:N2     | 23:DB:309:A:H3'    | 2.17                     | 0.58              |
| 23:DB:419:U:H2'    | 23:DB:420:C:C6     | 2.38                     | 0.58              |
| 23:DB:764:A:H5''   | 25:DC:208:GLY:HA3  | 1.84                     | 0.58              |
| 23:DB:946:C:H2'    | 23:DB:947:A:H8     | 1.68                     | 0.58              |
| 23:DB:1229:C:H2'   | 23:DB:1230:A:H8    | 1.68                     | 0.58              |
| 23:DB:1515:A:H4'   | 23:DB:1556:C:O2'   | 2.04                     | 0.58              |
| 23:DB:2783:U:H2'   | 23:DB:2784:U:H6    | 1.68                     | 0.58              |
| 25:DC:109:LEU:HD21 | 25:DC:115:ILE:HD11 | 1.84                     | 0.58              |
| 27:DE:14:VAL:HG12  | 27:DE:16:GLU:H     | 1.67                     | 0.58              |
| 30:DH:3:VAL:O      | 30:DH:18:GLN:HA    | 2.03                     | 0.58              |
| 30:DH:5:LEU:HD23   | 30:DH:17:ASP:O     | 2.02                     | 0.58              |
| 33:DL:7:SER:HB2    | 33:DL:8:PRO:CD     | 2.17                     | 0.58              |
| 37:DP:38:ARG:CG    | 37:DP:39:LEU:H     | 2.08                     | 0.58              |
| 38:DQ:39:ILE:O     | 38:DQ:43:GLN:HB3   | 2.02                     | 0.58              |
| 38:DQ:89:ILE:H     | 38:DQ:89:ILE:HD12  | 1.69                     | 0.58              |
| 39:DR:71:LYS:HB2   | 39:DR:73:LYS:NZ    | 2.18                     | 0.58              |
| 40:DS:8:ARG:O      | 40:DS:9:HIS:HB2    | 2.02                     | 0.58              |
| 42:DU:11:ILE:HB    | 42:DU:69:VAL:HG23  | 1.84                     | 0.58              |
| 52:DI:85:ILE:CD1   | 52:DI:137:LEU:HD21 | 2.32                     | 0.58              |
| 1:AA:88:U:O2'      | 1:AA:89:U:C6       | 2.56                     | 0.58              |
| 1:AA:621:A:H2'     | 1:AA:622:A:C8      | 2.38                     | 0.58              |
| 1:AA:1324:A:H2'    | 1:AA:1325:C:H6     | 1.69                     | 0.58              |
| 2:AC:100:ILE:C     | 2:AC:100:ILE:HD13  | 2.29                     | 0.58              |
| 2:AC:151:GLU:O     | 2:AC:197:VAL:HA    | 2.02                     | 0.58              |
| 10:AK:26:PHE:HE1   | 10:AK:88:PRO:HG2   | 1.68                     | 0.58              |
| 11:AL:22:ALA:HB2   | 11:AL:56:LEU:HD21  | 1.85                     | 0.58              |
| 16:AQ:66:LEU:HD11  | 16:AQ:73:THR:HG22  | 1.85                     | 0.58              |
| 23:BB:27:G:N2      | 23:BB:512:G:H2'    | 2.17                     | 0.58              |
| 23:BB:111:A:H2'    | 23:BB:112:U:O4'    | 2.02                     | 0.58              |
| 23:BB:794:A:H2'    | 23:BB:795:C:H6     | 1.67                     | 0.58              |
| 23:BB:1082:U:N3    | 23:BB:1086:A:C2    | 2.71                     | 0.58              |
| 23:BB:1144:A:O2'   | 23:BB:1145:C:H5'   | 2.03                     | 0.58              |
| 23:BB:1229:C:H2'   | 23:BB:1230:A:C8    | 2.38                     | 0.58              |
| 23:BB:2898:U:H2'   | 23:BB:2899:A:H8    | 1.69                     | 0.58              |
| 25:BC:119:VAL:HG13 | 25:BC:133:ASN:ND2  | 2.18                     | 0.58              |
| 25:BC:181:ARG:NH1  | 25:BC:260:LYS:HD2  | 2.18                     | 0.58              |
| 26:BD:83:ARG:HH12  | 26:BD:85:ALA:HB2   | 1.67                     | 0.58              |
| 27:BE:198:GLU:C    | 27:BE:200:LEU:H    | 2.12                     | 0.58              |
| 40:BS:50:VAL:HG11  | 40:BS:103:ILE:HG12 | 1.85                     | 0.58              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:BW:40:ARG:HH12  | 43:BW:68:PHE:HA    | 1.67                     | 0.58              |
| 51:B4:16:ILE:HD12  | 51:B4:16:ILE:H     | 1.68                     | 0.58              |
| 1:CA:241:G:O2'     | 1:CA:242:G:H5'     | 2.02                     | 0.58              |
| 1:CA:620:C:C2      | 3:CD:131:ILE:HD13  | 2.38                     | 0.58              |
| 4:CE:104:ILE:HG23  | 4:CE:104:ILE:O     | 2.03                     | 0.58              |
| 6:CG:37:THR:O      | 6:CG:41:ILE:HG13   | 2.03                     | 0.58              |
| 8:CI:50:PRO:HD3    | 8:CI:79:ARG:HD3    | 1.85                     | 0.58              |
| 10:CK:28:ASN:ND2   | 10:CK:29:THR:H     | 2.00                     | 0.58              |
| 23:DB:69:C:H2'     | 23:DB:70:G:H8      | 1.68                     | 0.58              |
| 23:DB:90:U:H2'     | 23:DB:91:A:C2      | 2.39                     | 0.58              |
| 23:DB:125:A:H4'    | 49:D2:13:ASN:ND2   | 2.18                     | 0.58              |
| 23:DB:942:G:O2'    | 23:DB:943:A:H5'    | 2.03                     | 0.58              |
| 23:DB:1579:A:H2'   | 23:DB:1580:A:C8    | 2.38                     | 0.58              |
| 23:DB:2756:U:C1'   | 23:DB:2757:A:H5''  | 2.34                     | 0.58              |
| 24:DV:43:ASP:OD2   | 24:DV:46:LYS:HB2   | 2.03                     | 0.58              |
| 25:DC:28:PRO:HG2   | 25:DC:79:ARG:NH2   | 2.18                     | 0.58              |
| 26:DD:24:VAL:CG1   | 26:DD:193:VAL:HG21 | 2.34                     | 0.58              |
| 26:DD:153:GLY:C    | 26:DD:155:VAL:H    | 2.11                     | 0.58              |
| 29:DG:70:LEU:O     | 29:DG:74:MET:HG3   | 2.03                     | 0.58              |
| 29:DG:156:TYR:HA   | 29:DG:171:LYS:HG3  | 1.84                     | 0.58              |
| 30:DH:115:VAL:HB   | 30:DH:132:PHE:HD1  | 1.68                     | 0.58              |
| 30:DH:135:HIS:HB3  | 30:DH:138:VAL:CG2  | 2.33                     | 0.58              |
| 34:DM:16:ARG:NH2   | 34:DM:72:PRO:HG2   | 2.17                     | 0.58              |
| 38:DQ:15:LYS:O     | 38:DQ:19:GLN:HG2   | 2.03                     | 0.58              |
| 39:DR:6:GLN:HB3    | 39:DR:41:ILE:HD13  | 1.84                     | 0.58              |
| 42:DU:32:LYS:HA    | 42:DU:65:GLN:HE21  | 1.68                     | 0.58              |
| 1:AA:186:C:H4'     | 19:AT:75:LYS:HB2   | 1.85                     | 0.58              |
| 1:AA:476:U:H2'     | 1:AA:477:C:C6      | 2.38                     | 0.58              |
| 2:AC:5:HIS:CD2     | 2:AC:7:ASN:HB2     | 2.38                     | 0.58              |
| 20:AB:172:ILE:HG22 | 20:AB:176:ASN:HD21 | 1.68                     | 0.58              |
| 23:BB:172:A:H2'    | 23:BB:173:A:H8     | 1.68                     | 0.58              |
| 23:BB:917:A:C2     | 23:BB:918:A:H1'    | 2.38                     | 0.58              |
| 23:BB:1259:G:H2'   | 23:BB:1260:A:H8    | 1.68                     | 0.58              |
| 23:BB:1537:G:H3'   | 23:BB:1537:G:N3    | 2.18                     | 0.58              |
| 23:BB:1777:U:O2'   | 23:BB:1778:U:H5'   | 2.03                     | 0.58              |
| 23:BB:2267:A:N6    | 23:BB:2272:U:C4    | 2.67                     | 0.58              |
| 23:BB:2491:U:H5''  | 23:BB:2570:G:H5''  | 1.85                     | 0.58              |
| 23:BB:2811:G:OP1   | 26:BD:61:THR:HB    | 2.04                     | 0.58              |
| 23:BB:2873:A:N3    | 35:BN:6:SER:HA     | 2.18                     | 0.58              |
| 24:BV:42:LEU:HB2   | 24:BV:47:VAL:HG21  | 1.85                     | 0.58              |
| 27:BE:38:GLY:C     | 27:BE:40:ARG:H     | 2.09                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:BF:107:VAL:N    | 28:BF:108:PRO:CD   | 2.65                     | 0.58              |
| 33:BL:64:PHE:CD1   | 50:B3:24:LYS:HE3   | 2.39                     | 0.58              |
| 33:BL:84:LYS:O     | 33:BL:85:VAL:HG12  | 2.03                     | 0.58              |
| 39:BR:20:VAL:HG13  | 39:BR:97:LYS:HZ2   | 1.68                     | 0.58              |
| 41:BT:25:GLU:HG3   | 41:BT:26:LYS:H     | 1.67                     | 0.58              |
| 42:BU:71:ILE:HD13  | 42:BU:72:PHE:O     | 2.03                     | 0.58              |
| 1:CA:1021:A:H2'    | 1:CA:1022:A:C8     | 2.38                     | 0.58              |
| 11:CL:77:SER:O     | 11:CL:79:ILE:HG23  | 2.03                     | 0.58              |
| 13:CN:62:ARG:N     | 13:CN:72:PHE:HZ    | 2.02                     | 0.58              |
| 14:CO:62:ARG:CZ    | 14:CO:86:LEU:HD21  | 2.33                     | 0.58              |
| 23:DB:208:C:H2'    | 23:DB:209:C:H6     | 1.68                     | 0.58              |
| 23:DB:2010:G:H5''  | 40:DS:42:LYS:HB2   | 1.84                     | 0.58              |
| 23:DB:2421:G:OP2   | 50:D3:31:ILE:HG21  | 2.04                     | 0.58              |
| 23:DB:2491:U:H5''  | 23:DB:2570:G:H5''  | 1.85                     | 0.58              |
| 23:DB:2893:A:H5''  | 23:DB:2894:G:H5'   | 1.85                     | 0.58              |
| 25:DC:110:LYS:HA   | 25:DC:110:LYS:HE3  | 1.84                     | 0.58              |
| 27:DE:147:LEU:H    | 27:DE:147:LEU:HD12 | 1.68                     | 0.58              |
| 27:DE:151:GLY:O    | 27:DE:171:ASP:HA   | 2.04                     | 0.58              |
| 27:DE:187:VAL:HG23 | 27:DE:188:MET:H    | 1.68                     | 0.58              |
| 32:DK:6:THR:HG22   | 32:DK:7:MET:H      | 1.68                     | 0.58              |
| 32:DK:43:ILE:HD12  | 32:DK:43:ILE:N     | 2.18                     | 0.58              |
| 41:DT:87:LEU:HD22  | 41:DT:93:LEU:HD11  | 1.85                     | 0.58              |
| 44:DX:56:LEU:HA    | 44:DX:59:GLU:HB2   | 1.86                     | 0.58              |
| 49:D2:13:ASN:C     | 49:D2:15:SER:H     | 2.10                     | 0.58              |
| 51:D4:10:LEU:HB2   | 51:D4:25:VAL:CG2   | 2.34                     | 0.58              |
| 1:AA:922:G:N3      | 1:AA:1398:A:H2     | 2.02                     | 0.58              |
| 1:AA:923:A:H2'     | 1:AA:924:C:C6      | 2.39                     | 0.58              |
| 1:AA:1366:C:H2'    | 1:AA:1367:C:H6     | 1.68                     | 0.58              |
| 1:AA:1508:A:H2'    | 1:AA:1509:C:C6     | 2.38                     | 0.58              |
| 14:AO:68:TYR:CZ    | 14:AO:72:LYS:HG3   | 2.39                     | 0.58              |
| 23:BB:26:G:H2'     | 23:BB:27:G:C1'     | 2.34                     | 0.58              |
| 23:BB:38:A:C8      | 27:BE:46:GLN:OE1   | 2.57                     | 0.58              |
| 23:BB:950:G:H2'    | 23:BB:951:C:C6     | 2.39                     | 0.58              |
| 23:BB:1046:A:C3'   | 23:BB:1047:G:H5''  | 2.32                     | 0.58              |
| 23:BB:1709:U:H2'   | 23:BB:1710:G:H8    | 1.68                     | 0.58              |
| 23:BB:1742:U:H2'   | 23:BB:1743:G:C8    | 2.38                     | 0.58              |
| 23:BB:1799:G:C5    | 25:BC:175:LEU:HD13 | 2.39                     | 0.58              |
| 23:BB:2083:G:H2'   | 23:BB:2084:C:C6    | 2.38                     | 0.58              |
| 26:BD:14:ILE:HA    | 26:BD:19:GLY:HA2   | 1.85                     | 0.58              |
| 26:BD:159:LYS:HB2  | 26:BD:159:LYS:HZ2  | 1.66                     | 0.58              |
| 30:BH:57:LYS:HG3   | 30:BH:61:VAL:CG2   | 2.34                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:BL:54:GLN:HB3   | 33:BL:56:PRO:HD2   | 1.84                     | 0.58              |
| 33:BL:78:ARG:CZ    | 33:BL:110:VAL:HG11 | 2.33                     | 0.58              |
| 39:BR:20:VAL:HG13  | 39:BR:97:LYS:HD2   | 1.86                     | 0.58              |
| 50:B3:12:ARG:HG2   | 50:B3:23:HIS:HB3   | 1.85                     | 0.58              |
| 1:CA:202:G:H2'     | 1:CA:203:G:H8      | 1.69                     | 0.58              |
| 1:CA:1320:C:H41    | 18:CS:36:ARG:HD2   | 1.68                     | 0.58              |
| 3:CD:36:ALA:C      | 3:CD:38:GLY:H      | 2.11                     | 0.58              |
| 23:DB:98:G:C3'     | 23:DB:99:U:H5''    | 2.33                     | 0.58              |
| 23:DB:1444:G:H2'   | 23:DB:1445:G:H8    | 1.67                     | 0.58              |
| 23:DB:1484:U:H2'   | 23:DB:1485:U:H6    | 1.68                     | 0.58              |
| 23:DB:1557:C:H3'   | 23:DB:1558:C:H5''  | 1.84                     | 0.58              |
| 23:DB:1777:U:O2'   | 23:DB:1778:U:H5'   | 2.03                     | 0.58              |
| 23:DB:2491:U:H5''  | 23:DB:2570:G:C5'   | 2.33                     | 0.58              |
| 27:DE:130:LYS:HB2  | 27:DE:130:LYS:HZ3  | 1.69                     | 0.58              |
| 31:DJ:94:ALA:HB1   | 31:DJ:95:ARG:HH21  | 1.69                     | 0.58              |
| 37:DP:71:ARG:HH11  | 37:DP:71:ARG:HB3   | 1.67                     | 0.58              |
| 1:AA:398:U:H2'     | 1:AA:399:G:C8      | 2.39                     | 0.58              |
| 1:AA:1100:C:OP2    | 20:AB:94:ARG:HD3   | 2.04                     | 0.58              |
| 1:AA:1130:A:O2'    | 1:AA:1131:G:H5'    | 2.04                     | 0.58              |
| 2:AC:71:ARG:NH2    | 2:AC:74:ILE:HB     | 2.18                     | 0.58              |
| 3:AD:17:ASP:OD2    | 3:AD:27:ILE:HG12   | 2.04                     | 0.58              |
| 3:AD:60:VAL:HB     | 3:AD:194:ILE:HG13  | 1.84                     | 0.58              |
| 4:AE:158:LYS:HE2   | 4:AE:158:LYS:N     | 2.19                     | 0.58              |
| 8:AI:91:GLU:CD     | 8:AI:94:ARG:HH21   | 2.11                     | 0.58              |
| 9:AJ:71:LEU:H      | 9:AJ:71:LEU:HD12   | 1.68                     | 0.58              |
| 23:BB:3:U:O2'      | 23:BB:4:U:H6       | 1.87                     | 0.58              |
| 23:BB:19:A:H2'     | 23:BB:20:C:H6      | 1.65                     | 0.58              |
| 23:BB:21:A:O2'     | 23:BB:22:C:H5'     | 2.04                     | 0.58              |
| 23:BB:146:A:H2'    | 23:BB:147:C:H6     | 1.66                     | 0.58              |
| 23:BB:1847:A:H4'   | 23:BB:1848:A:C8    | 2.39                     | 0.58              |
| 23:BB:1932:A:H2'   | 23:BB:1933:G:O4'   | 2.04                     | 0.58              |
| 23:BB:2351:G:O6    | 50:B3:38:LYS:HD2   | 2.03                     | 0.58              |
| 25:BC:75:ALA:HB2   | 25:BC:95:TYR:CE1   | 2.38                     | 0.58              |
| 26:BD:138:LEU:HD23 | 26:BD:139:SER:H    | 1.68                     | 0.58              |
| 27:BE:144:GLU:C    | 27:BE:146:VAL:H    | 2.11                     | 0.58              |
| 33:BL:133:ALA:HA   | 33:BL:136:GLU:OE2  | 2.03                     | 0.58              |
| 34:BM:3:GLN:O      | 34:BM:4:PRO:C      | 2.46                     | 0.58              |
| 34:BM:11:LYS:O     | 34:BM:12:MET:HE2   | 2.03                     | 0.58              |
| 34:BM:67:VAL:HB    | 34:BM:100:LYS:CG   | 2.32                     | 0.58              |
| 35:BN:29:VAL:HG22  | 35:BN:83:LEU:HD22  | 1.85                     | 0.58              |
| 36:BO:8:ILE:C      | 36:BO:10:ARG:H     | 2.12                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BO:21:LEU:HD13  | 36:BO:22:GLY:N     | 2.18                     | 0.58              |
| 36:BO:40:ILE:HG12  | 36:BO:41:ALA:O     | 2.04                     | 0.58              |
| 1:CA:26:A:N6       | 1:CA:558:G:H1'     | 2.19                     | 0.58              |
| 1:CA:212:G:H2'     | 1:CA:213:G:H8      | 1.68                     | 0.58              |
| 1:CA:1142:G:H2'    | 1:CA:1143:G:H8     | 1.68                     | 0.58              |
| 1:CA:1299:A:N7     | 1:CA:1301:U:H1'    | 2.19                     | 0.58              |
| 12:CM:79:LEU:HA    | 12:CM:82:LEU:HG    | 1.85                     | 0.58              |
| 22:DA:28:C:OP1     | 36:DO:33:ARG:HD3   | 2.04                     | 0.58              |
| 22:DA:35:C:H2'     | 22:DA:36:C:O4'     | 2.03                     | 0.58              |
| 23:DB:138:U:H2'    | 23:DB:140:C:C6     | 2.38                     | 0.58              |
| 23:DB:479:A:N3     | 23:DB:481:G:H5''   | 2.19                     | 0.58              |
| 23:DB:976:G:H4'    | 23:DB:1156:A:N7    | 2.19                     | 0.58              |
| 23:DB:1439:A:N6    | 23:DB:1440:U:O2    | 2.35                     | 0.58              |
| 23:DB:2020:A:H5'   | 47:D0:8:THR:HG21   | 1.84                     | 0.58              |
| 23:DB:2024:G:H5''  | 26:DD:154:LYS:NZ   | 2.18                     | 0.58              |
| 23:DB:2466:C:OP1   | 51:D4:5:ALA:HB3    | 2.04                     | 0.58              |
| 25:DC:74:PRO:HG3   | 25:DC:116:GLN:HG2  | 1.85                     | 0.58              |
| 28:DF:56:LEU:HA    | 28:DF:59:ILE:CG2   | 2.34                     | 0.58              |
| 29:DG:171:LYS:HD3  | 29:DG:172:GLU:C    | 2.29                     | 0.58              |
| 33:DL:90:VAL:HG13  | 33:DL:122:VAL:HG13 | 1.86                     | 0.58              |
| 41:DT:34:VAL:HG22  | 41:DT:35:ALA:H     | 1.67                     | 0.58              |
| 41:DT:66:LYS:HA    | 41:DT:76:ARG:O     | 2.03                     | 0.58              |
| 1:AA:742:G:O2'     | 1:AA:743:A:H5'     | 2.03                     | 0.58              |
| 1:AA:1160:G:H2'    | 1:AA:1161:C:H6     | 1.69                     | 0.58              |
| 1:AA:1299:A:H62    | 1:AA:1302:C:H5     | 1.52                     | 0.58              |
| 2:AC:113:LYS:HD2   | 2:AC:184:ASN:OD1   | 2.04                     | 0.58              |
| 3:AD:177:MET:HE2   | 3:AD:177:MET:H     | 1.69                     | 0.58              |
| 3:AD:191:SER:O     | 3:AD:192:ALA:HB2   | 2.04                     | 0.58              |
| 4:AE:140:ILE:HA    | 4:AE:143:LEU:HD12  | 1.85                     | 0.58              |
| 10:AK:110:THR:HG22 | 21:AU:4:LYS:HA     | 1.86                     | 0.58              |
| 16:AQ:23:ALA:C     | 16:AQ:24:ILE:HD12  | 2.29                     | 0.58              |
| 20:AB:65:LYS:HD2   | 20:AB:157:PRO:HA   | 1.86                     | 0.58              |
| 20:AB:166:ASP:OD1  | 20:AB:190:SER:HA   | 2.03                     | 0.58              |
| 20:AB:187:ASP:HB2  | 20:AB:203:ASP:HB3  | 1.86                     | 0.58              |
| 23:BB:17:G:H2'     | 23:BB:18:U:C6      | 2.39                     | 0.58              |
| 23:BB:55:G:P       | 49:B2:35:ARG:HH21  | 2.26                     | 0.58              |
| 23:BB:782:A:O2'    | 25:BC:223:ALA:HB1  | 2.04                     | 0.58              |
| 23:BB:950:G:H2'    | 23:BB:951:C:H6     | 1.67                     | 0.58              |
| 23:BB:962:G:N2     | 34:BM:81:ARG:HH21  | 2.01                     | 0.58              |
| 23:BB:1199:U:H2'   | 23:BB:1200:C:H6    | 1.67                     | 0.58              |
| 23:BB:1791:A:C2    | 23:BB:1829:A:C4'   | 2.87                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BB:2874:C:P    | 35:BN:5:LYS:HG2   | 2.44                     | 0.58              |
| 26:BD:157:LYS:HG2 | 31:BJ:79:GLY:O    | 2.02                     | 0.58              |
| 29:BG:60:GLY:O    | 29:BG:63:GLN:HG2  | 2.04                     | 0.58              |
| 32:BK:40:LYS:NZ   | 32:BK:89:ASN:HD21 | 2.01                     | 0.58              |
| 33:BL:57:LEU:O    | 33:BL:57:LEU:HD12 | 2.03                     | 0.58              |
| 37:BP:7:LEU:HD13  | 37:BP:11:GLN:HG2  | 1.84                     | 0.58              |
| 40:BS:29:VAL:CG2  | 40:BS:71:VAL:HG23 | 2.34                     | 0.58              |
| 45:BY:22:THR:HG21 | 45:BY:50:VAL:HG11 | 1.85                     | 0.58              |
| 46:BZ:5:ILE:H     | 46:BZ:5:ILE:CD1   | 2.11                     | 0.58              |
| 1:CA:450:G:N7     | 1:CA:481:G:O6     | 2.37                     | 0.58              |
| 1:CA:797:C:OP1    | 10:CK:125:LYS:HG3 | 2.04                     | 0.58              |
| 1:CA:1219:A:H2'   | 1:CA:1220:G:C8    | 2.39                     | 0.58              |
| 1:CA:1323:G:H2'   | 1:CA:1324:A:H8    | 1.68                     | 0.58              |
| 3:CD:19:PHE:O     | 3:CD:22:SER:HB2   | 2.03                     | 0.58              |
| 10:CK:70:ALA:C    | 10:CK:72:ALA:H    | 2.11                     | 0.58              |
| 11:CL:80:LEU:HD23 | 11:CL:97:VAL:HG21 | 1.86                     | 0.58              |
| 16:CQ:10:ARG:NH2  | 16:CQ:55:GLY:N    | 2.52                     | 0.58              |
| 17:CR:23:LYS:O    | 17:CR:23:LYS:HD2  | 2.04                     | 0.58              |
| 22:DA:102:G:H2'   | 22:DA:103:U:C6    | 2.39                     | 0.58              |
| 25:DC:21:PRO:HG2  | 25:DC:22:GLU:H    | 1.68                     | 0.58              |
| 26:DD:148:GLN:HB3 | 26:DD:151:THR:CG2 | 2.34                     | 0.58              |
| 27:DE:115:GLN:CG  | 27:DE:116:ASP:H   | 2.17                     | 0.58              |
| 27:DE:152:GLU:HB2 | 27:DE:158:PHE:CE1 | 2.38                     | 0.58              |
| 30:DH:94:ILE:CG2  | 30:DH:122:LEU:HG  | 2.33                     | 0.58              |
| 34:DM:81:ARG:HG3  | 34:DM:82:MET:HG2  | 1.85                     | 0.58              |
| 35:DN:35:LYS:HD3  | 35:DN:112:TYR:CD1 | 2.39                     | 0.58              |
| 38:DQ:109:VAL:O   | 38:DQ:113:LYS:HB2 | 2.04                     | 0.58              |
| 40:DS:2:GLU:HB2   | 40:DS:108:SER:HA  | 1.85                     | 0.58              |
| 40:DS:39:THR:O    | 40:DS:39:THR:HG23 | 2.03                     | 0.58              |
| 42:DU:8:ASP:O     | 42:DU:10:VAL:N    | 2.37                     | 0.58              |
| 43:DW:44:PHE:CE2  | 43:DW:60:ALA:HB2  | 2.38                     | 0.58              |
| 45:DY:38:GLU:O    | 45:DY:43:ILE:HG21 | 2.04                     | 0.58              |
| 46:DZ:11:GLU:H    | 46:DZ:27:THR:CG2  | 2.16                     | 0.58              |
| 47:D0:27:LEU:H    | 47:D0:27:LEU:CD2  | 2.15                     | 0.58              |
| 50:D3:12:ARG:NE   | 50:D3:23:HIS:HB2  | 2.19                     | 0.58              |
| 52:DI:76:ALA:HA   | 52:DI:135:MET:SD  | 2.44                     | 0.58              |
| 1:AA:26:A:N6      | 1:AA:558:G:H1'    | 2.19                     | 0.58              |
| 1:AA:80:A:H2'     | 1:AA:81:A:O4'     | 2.04                     | 0.58              |
| 1:AA:1171:A:H2'   | 1:AA:1172:C:C6    | 2.38                     | 0.58              |
| 1:AA:1468:A:H2'   | 1:AA:1469:C:O4'   | 2.03                     | 0.58              |
| 1:AA:1519:A:H3'   | 1:AA:1520:C:C5'   | 2.34                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:AD:138:PRO:HA    | 3:AD:181:PHE:CD2  | 2.39                     | 0.58              |
| 4:AE:13:LYS:HE3    | 4:AE:115:GLU:HB2  | 1.86                     | 0.58              |
| 4:AE:111:ARG:O     | 4:AE:115:GLU:HG3  | 2.04                     | 0.58              |
| 5:AF:64:VAL:HG12   | 5:AF:65:GLU:N     | 2.15                     | 0.58              |
| 8:AI:51:LEU:HB3    | 8:AI:56:MET:HG2   | 1.85                     | 0.58              |
| 9:AJ:40:ILE:HG22   | 9:AJ:41:PRO:HD2   | 1.86                     | 0.58              |
| 13:AN:63:CYS:SG    | 13:AN:66:THR:HG22 | 2.44                     | 0.58              |
| 23:BB:18:U:H2'     | 23:BB:19:A:C8     | 2.38                     | 0.58              |
| 23:BB:458:G:N2     | 23:BB:469:G:H2'   | 2.19                     | 0.58              |
| 23:BB:651:G:P      | 50:B3:16:THR:HB   | 2.44                     | 0.58              |
| 23:BB:705:A:N6     | 23:BB:726:G:O2'   | 2.37                     | 0.58              |
| 23:BB:1055:G:HO2'  | 23:BB:1085:A:H2   | 1.46                     | 0.58              |
| 23:BB:1722:A:H61   | 23:BB:1738:G:H1'  | 1.69                     | 0.58              |
| 23:BB:2105:U:H2'   | 23:BB:2106:U:C6   | 2.39                     | 0.58              |
| 23:BB:2378:A:H2'   | 23:BB:2379:G:H5'  | 1.85                     | 0.58              |
| 23:BB:2415:G:H2'   | 23:BB:2416:C:C6   | 2.39                     | 0.58              |
| 23:BB:2530:A:N6    | 29:BG:155:PRO:HG3 | 2.19                     | 0.58              |
| 23:BB:2572:A:C8    | 26:BD:150:GLN:O   | 2.57                     | 0.58              |
| 23:BB:2783:U:H2'   | 23:BB:2784:U:H6   | 1.68                     | 0.58              |
| 25:BC:63:ILE:O     | 25:BC:64:VAL:HG13 | 2.04                     | 0.58              |
| 27:BE:52:VAL:HG13  | 27:BE:53:THR:N    | 2.18                     | 0.58              |
| 28:BF:132:ARG:HH11 | 28:BF:132:ARG:HG3 | 1.68                     | 0.58              |
| 29:BG:49:LEU:HD12  | 29:BG:49:LEU:N    | 2.19                     | 0.58              |
| 30:BH:3:VAL:HG13   | 30:BH:21:VAL:HG11 | 1.86                     | 0.58              |
| 35:BN:116:VAL:HG13 | 35:BN:117:ASP:N   | 2.19                     | 0.58              |
| 41:BT:58:VAL:HG12  | 41:BT:59:ASN:H    | 1.68                     | 0.58              |
| 46:BZ:25:ARG:HH11  | 46:BZ:25:ARG:CB   | 2.11                     | 0.58              |
| 1:CA:398:U:H2'     | 1:CA:399:G:C8     | 2.39                     | 0.58              |
| 1:CA:687:A:C2      | 1:CA:704:A:C5     | 2.91                     | 0.58              |
| 1:CA:865:A:H2'     | 1:CA:866:C:H6     | 1.68                     | 0.58              |
| 1:CA:1200:C:C3'    | 1:CA:1201:A:H5'   | 2.33                     | 0.58              |
| 2:CC:129:PHE:CE2   | 2:CC:156:LEU:HD13 | 2.38                     | 0.58              |
| 6:CG:74:VAL:HG21   | 6:CG:143:MET:HG2  | 1.86                     | 0.58              |
| 7:CH:77:VAL:HG23   | 7:CH:126:CYS:HA   | 1.85                     | 0.58              |
| 15:CP:44:SER:C     | 15:CP:46:LYS:H    | 2.12                     | 0.58              |
| 19:CT:43:LYS:HB3   | 19:CT:86:ALA:HB3  | 1.84                     | 0.58              |
| 23:DB:267:C:H2'    | 23:DB:268:C:H6    | 1.69                     | 0.58              |
| 23:DB:331:C:O2'    | 23:DB:332:A:H5'   | 2.04                     | 0.58              |
| 23:DB:499:U:H2'    | 23:DB:500:G:O4'   | 2.04                     | 0.58              |
| 23:DB:634:C:H2'    | 23:DB:635:C:H6    | 1.68                     | 0.58              |
| 23:DB:936:A:H2'    | 23:DB:937:C:H6    | 1.68                     | 0.58              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:1439:A:N7   | 23:DB:1440:U:N1    | 2.51                     | 0.58              |
| 23:DB:2257:U:H5'  | 43:DW:5:ALA:CB     | 2.34                     | 0.58              |
| 23:DB:2415:G:H2'  | 23:DB:2416:C:C6    | 2.39                     | 0.58              |
| 23:DB:2820:A:H4'  | 35:DN:4:ARG:HG3    | 1.84                     | 0.58              |
| 27:DE:193:VAL:HA  | 27:DE:198:GLU:C    | 2.28                     | 0.58              |
| 31:DJ:7:LYS:HD2   | 31:DJ:45:THR:OG1   | 2.04                     | 0.58              |
| 36:DO:75:GLY:HA3  | 36:DO:109:ALA:HB3  | 1.86                     | 0.58              |
| 42:DU:57:ILE:HD13 | 42:DU:57:ILE:C     | 2.29                     | 0.58              |
| 1:AA:8:A:H1'      | 4:AE:107:GLY:HA2   | 1.86                     | 0.58              |
| 1:AA:501:C:H1'    | 1:AA:549:C:H1'     | 1.85                     | 0.58              |
| 1:AA:552:U:H2'    | 1:AA:553:A:H8      | 1.69                     | 0.58              |
| 1:AA:1060:U:H5''  | 9:AJ:53:ILE:CG2    | 2.34                     | 0.58              |
| 1:AA:1434:A:H2'   | 1:AA:1435:G:C8     | 2.39                     | 0.58              |
| 4:AE:85:LYS:HE2   | 4:AE:92:ARG:HH11   | 1.68                     | 0.58              |
| 6:AG:144:ALA:C    | 6:AG:146:ALA:H     | 2.11                     | 0.58              |
| 8:AI:21:LYS:O     | 8:AI:60:LEU:HB2    | 2.03                     | 0.58              |
| 9:AJ:31:ARG:HG2   | 9:AJ:31:ARG:NH1    | 2.19                     | 0.58              |
| 15:AP:41:PRO:O    | 15:AP:42:ILE:HD13  | 2.03                     | 0.58              |
| 20:AB:163:ILE:O   | 20:AB:185:ILE:HG13 | 2.04                     | 0.58              |
| 23:BB:11:C:H2'    | 23:BB:12:U:H5'     | 1.85                     | 0.58              |
| 23:BB:660:C:H2'   | 23:BB:661:A:C8     | 2.39                     | 0.58              |
| 26:BD:8:LYS:HD2   | 37:BP:5:LYS:HD2    | 1.85                     | 0.58              |
| 28:BF:65:LEU:C    | 28:BF:67:THR:H     | 2.11                     | 0.58              |
| 32:BK:108:ARG:HB2 | 32:BK:116:ILE:HD13 | 1.84                     | 0.58              |
| 35:BN:67:PHE:HD2  | 35:BN:73:ASN:HD21  | 1.52                     | 0.58              |
| 36:BO:9:ARG:HA    | 36:BO:12:THR:HG23  | 1.85                     | 0.58              |
| 41:BT:11:LEU:HB2  | 41:BT:32:LEU:HD23  | 1.85                     | 0.58              |
| 41:BT:39:THR:O    | 41:BT:43:ILE:HG12  | 2.03                     | 0.58              |
| 42:BU:40:LEU:HD13 | 42:BU:41:VAL:H     | 1.69                     | 0.58              |
| 44:BX:2:LYS:H     | 44:BX:2:LYS:HD2    | 1.69                     | 0.58              |
| 44:BX:22:LEU:HA   | 44:BX:47:ARG:HH22  | 1.68                     | 0.58              |
| 52:BI:11:GLN:O    | 52:BI:11:GLN:HG3   | 2.03                     | 0.58              |
| 1:CA:677:U:H2'    | 1:CA:678:U:H6      | 1.69                     | 0.58              |
| 1:CA:801:U:H2'    | 1:CA:802:A:H8      | 1.68                     | 0.58              |
| 1:CA:1036:A:H2'   | 1:CA:1037:C:H6     | 1.68                     | 0.58              |
| 1:CA:1387:G:H2'   | 1:CA:1388:C:C6     | 2.38                     | 0.58              |
| 6:CG:12:LEU:HD13  | 6:CG:13:PRO:HD2    | 1.85                     | 0.58              |
| 14:CO:88:ARG:NH2  | 23:DB:714:U:H3'    | 2.19                     | 0.58              |
| 21:CU:25:ALA:C    | 21:CU:27:VAL:H     | 2.10                     | 0.58              |
| 23:DB:225:C:H2'   | 23:DB:226:A:O4'    | 2.03                     | 0.58              |
| 23:DB:1537:G:H3'  | 23:DB:1537:G:N3    | 2.19                     | 0.58              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:1818:U:H2'   | 25:DC:152:GLN:O    | 2.04                     | 0.58              |
| 23:DB:1847:A:H4'   | 23:DB:1848:A:C8    | 2.39                     | 0.58              |
| 23:DB:2839:G:C4'   | 35:DN:49:GLU:HG2   | 2.32                     | 0.58              |
| 25:DC:173:LEU:HD12 | 25:DC:183:VAL:HG11 | 1.86                     | 0.58              |
| 26:DD:23:PRO:HB3   | 26:DD:188:LEU:HB3  | 1.84                     | 0.58              |
| 26:DD:116:LYS:HB2  | 26:DD:165:MET:HB2  | 1.86                     | 0.58              |
| 27:DE:4:VAL:HG13   | 27:DE:5:LEU:N      | 2.14                     | 0.58              |
| 27:DE:172:ALA:O    | 27:DE:173:THR:HG22 | 2.04                     | 0.58              |
| 29:DG:5:LYS:HD3    | 29:DG:68:ARG:CB    | 2.33                     | 0.58              |
| 30:DH:1:MET:O      | 30:DH:21:VAL:HG22  | 2.01                     | 0.58              |
| 31:DJ:25:LEU:HD12  | 31:DJ:62:VAL:HA    | 1.86                     | 0.58              |
| 31:DJ:81:ILE:HG23  | 31:DJ:82:GLY:N     | 2.12                     | 0.58              |
| 44:DX:49:ASP:HA    | 44:DX:52:ARG:NH1   | 2.19                     | 0.58              |
| 49:D2:16:HIS:NE2   | 49:D2:44:VAL:HA    | 2.19                     | 0.58              |
| 50:D3:49:VAL:HG13  | 50:D3:51:LYS:H     | 1.69                     | 0.58              |
| 1:AA:537:G:H5''    | 11:AL:109:ARG:NH1  | 2.19                     | 0.57              |
| 5:AF:40:GLU:HG3    | 5:AF:42:TRP:NE1    | 2.19                     | 0.57              |
| 16:AQ:23:ALA:HB1   | 16:AQ:40:THR:HG23  | 1.84                     | 0.57              |
| 22:BA:32:U:H1'     | 22:BA:52:A:N7      | 2.20                     | 0.57              |
| 23:BB:705:A:N6     | 23:BB:726:G:H1'    | 2.19                     | 0.57              |
| 23:BB:718:A:H5''   | 23:BB:719:C:H5     | 1.69                     | 0.57              |
| 23:BB:1163:G:O2'   | 23:BB:1164:C:H5'   | 2.04                     | 0.57              |
| 23:BB:1203:U:H3'   | 23:BB:1204:A:C5'   | 2.33                     | 0.57              |
| 23:BB:1439:A:N7    | 23:BB:1440:U:N1    | 2.51                     | 0.57              |
| 23:BB:1442:U:H2'   | 23:BB:1443:U:H6    | 1.69                     | 0.57              |
| 23:BB:1515:A:H4'   | 23:BB:1556:C:O2'   | 2.04                     | 0.57              |
| 23:BB:1818:U:H5''  | 25:BC:155:ARG:CG   | 2.34                     | 0.57              |
| 23:BB:1946:U:H2'   | 23:BB:1947:C:H6    | 1.69                     | 0.57              |
| 27:BE:43:THR:HG23  | 27:BE:44:ARG:NE    | 2.19                     | 0.57              |
| 27:BE:150:THR:HA   | 27:BE:187:VAL:HG23 | 1.85                     | 0.57              |
| 29:BG:20:GLY:HA2   | 29:BG:41:GLU:HG2   | 1.86                     | 0.57              |
| 30:BH:11:ASN:ND2   | 30:BH:12:LEU:H     | 2.01                     | 0.57              |
| 31:BJ:10:THR:HB    | 31:BJ:13:ARG:HH12  | 1.68                     | 0.57              |
| 33:BL:82:LEU:HD13  | 33:BL:83:ALA:N     | 2.19                     | 0.57              |
| 34:BM:64:TRP:O     | 34:BM:102:LEU:HB2  | 2.03                     | 0.57              |
| 42:BU:12:VAL:HG11  | 42:BU:18:LYS:H     | 1.67                     | 0.57              |
| 42:BU:71:ILE:HD13  | 42:BU:71:ILE:C     | 2.29                     | 0.57              |
| 46:BZ:63:ARG:CZ    | 46:BZ:63:ARG:HA    | 2.34                     | 0.57              |
| 1:CA:335:C:H2'     | 1:CA:336:A:C8      | 2.39                     | 0.57              |
| 1:CA:1072:G:H2'    | 1:CA:1073:U:H6     | 1.69                     | 0.57              |
| 1:CA:1096:C:H2'    | 1:CA:1097:C:H6     | 1.67                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:CN:40:ARG:HH11  | 13:CN:40:ARG:HG3   | 1.69                     | 0.57              |
| 15:CP:1:MET:HB3    | 15:CP:24:SER:OG    | 2.04                     | 0.57              |
| 20:CB:57:ASN:ND2   | 20:CB:223:GLY:HA2  | 2.19                     | 0.57              |
| 20:CB:202:ASN:ND2  | 20:CB:203:ASP:N    | 2.51                     | 0.57              |
| 21:CU:3:ILE:HG12   | 21:CU:19:LYS:HB3   | 1.85                     | 0.57              |
| 23:DB:125:A:H4'    | 49:D2:13:ASN:HD21  | 1.69                     | 0.57              |
| 23:DB:1552:A:C2'   | 23:DB:1553:A:H5'   | 2.33                     | 0.57              |
| 23:DB:2072:C:H2'   | 23:DB:2073:C:H6    | 1.69                     | 0.57              |
| 23:DB:2553:G:H2'   | 23:DB:2554:U:C4'   | 2.34                     | 0.57              |
| 23:DB:2567:G:H2'   | 23:DB:2568:U:C6    | 2.39                     | 0.57              |
| 23:DB:2650:U:H2'   | 23:DB:2651:C:H6    | 1.69                     | 0.57              |
| 25:DC:53:ILE:HG21  | 25:DC:218:THR:OG1  | 2.04                     | 0.57              |
| 27:DE:141:MET:HB3  | 27:DE:185:LYS:HZ1  | 1.68                     | 0.57              |
| 29:DG:85:LYS:HB3   | 29:DG:131:VAL:HA   | 1.85                     | 0.57              |
| 32:DK:105:ARG:HD3  | 32:DK:105:ARG:H    | 1.68                     | 0.57              |
| 36:DO:27:VAL:HG23  | 36:DO:28:VAL:H     | 1.67                     | 0.57              |
| 36:DO:30:ARG:HD3   | 36:DO:30:ARG:N     | 2.19                     | 0.57              |
| 37:DP:27:VAL:HG23  | 37:DP:86:LYS:HB3   | 1.85                     | 0.57              |
| 40:DS:23:LEU:HB2   | 47:D0:21:LEU:CD1   | 2.30                     | 0.57              |
| 44:DX:1:MET:HB2    | 44:DX:6:LEU:HG     | 1.86                     | 0.57              |
| 49:D2:46:LYS:HE3   | 49:D2:46:LYS:O     | 2.04                     | 0.57              |
| 50:D3:2:LYS:HB2    | 50:D3:2:LYS:NZ     | 2.19                     | 0.57              |
| 51:D4:16:ILE:C     | 51:D4:18:LYS:H     | 2.12                     | 0.57              |
| 1:AA:16:A:HO2'     | 4:AE:20:VAL:HG13   | 1.69                     | 0.57              |
| 1:AA:1027:C:H2'    | 1:AA:1028:C:H6     | 1.68                     | 0.57              |
| 1:AA:1039:G:H2'    | 1:AA:1040:U:C6     | 2.39                     | 0.57              |
| 1:AA:1491:G:H5''   | 1:AA:1492:A:OP2    | 2.04                     | 0.57              |
| 2:AC:59:PRO:HG2    | 2:AC:60:ALA:H      | 1.69                     | 0.57              |
| 20:AB:67:LEU:HD22  | 20:AB:67:LEU:N     | 2.19                     | 0.57              |
| 23:BB:208:C:H2'    | 23:BB:209:C:H6     | 1.69                     | 0.57              |
| 23:BB:582:A:H2'    | 23:BB:583:G:H8     | 1.68                     | 0.57              |
| 23:BB:1123:C:H2'   | 23:BB:1124:G:H8    | 1.69                     | 0.57              |
| 23:BB:1275:A:C2'   | 23:BB:1276:A:H5'   | 2.34                     | 0.57              |
| 23:BB:2247:A:H2'   | 23:BB:2248:C:C6    | 2.39                     | 0.57              |
| 23:BB:2339:C:H2'   | 23:BB:2340:A:H8    | 1.69                     | 0.57              |
| 23:BB:2553:G:H2'   | 23:BB:2554:U:C4'   | 2.34                     | 0.57              |
| 27:BE:118:LEU:HD23 | 27:BE:118:LEU:N    | 2.17                     | 0.57              |
| 27:BE:121:VAL:HG12 | 27:BE:122:GLU:N    | 2.19                     | 0.57              |
| 28:BF:64:PRO:HA    | 28:BF:88:VAL:HG22  | 1.86                     | 0.57              |
| 30:BH:134:VAL:HG13 | 30:BH:135:HIS:N    | 2.14                     | 0.57              |
| 35:BN:41:ALA:HA    | 35:BN:113:ILE:HD11 | 1.87                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:BN:73:ASN:HA   | 35:BN:76:VAL:HG13 | 1.86                     | 0.57              |
| 40:BS:56:ALA:C    | 40:BS:58:ALA:H    | 2.12                     | 0.57              |
| 45:BY:4:ILE:HB    | 45:BY:39:ASP:HB3  | 1.86                     | 0.57              |
| 1:CA:546:A:P      | 3:CD:68:GLU:HB3   | 2.44                     | 0.57              |
| 1:CA:688:G:H5'    | 10:CK:48:GLY:HA2  | 1.85                     | 0.57              |
| 1:CA:1496:C:H4'   | 23:DB:1920:C:O2'  | 2.04                     | 0.57              |
| 7:CH:93:LYS:HG2   | 7:CH:96:ALA:HA    | 1.84                     | 0.57              |
| 9:CJ:36:VAL:HG13  | 9:CJ:76:ILE:CD1   | 2.34                     | 0.57              |
| 16:CQ:26:ARG:NH2  | 16:CQ:39:ARG:HG2  | 2.19                     | 0.57              |
| 23:DB:135:U:H2'   | 23:DB:136:G:C8    | 2.38                     | 0.57              |
| 23:DB:155:A:H2'   | 23:DB:156:A:H8    | 1.69                     | 0.57              |
| 23:DB:179:C:H2'   | 23:DB:180:G:O4'   | 2.03                     | 0.57              |
| 23:DB:526:A:N6    | 23:DB:2626:C:C4'  | 2.66                     | 0.57              |
| 23:DB:536:G:H5''  | 38:DQ:52:ARG:HH22 | 1.69                     | 0.57              |
| 23:DB:660:C:H2'   | 23:DB:661:A:H8    | 1.68                     | 0.57              |
| 23:DB:921:C:H2'   | 23:DB:922:C:H6    | 1.68                     | 0.57              |
| 23:DB:962:G:H21   | 23:DB:2250:G:H1   | 1.52                     | 0.57              |
| 23:DB:987:C:H2'   | 23:DB:988:A:O4'   | 2.04                     | 0.57              |
| 23:DB:1198:U:H4'  | 38:DQ:8:ILE:HD11  | 1.87                     | 0.57              |
| 23:DB:1275:A:C2'  | 23:DB:1276:A:H5'  | 2.33                     | 0.57              |
| 23:DB:1709:U:H2'  | 23:DB:1710:G:H8   | 1.68                     | 0.57              |
| 23:DB:1739:A:H2'  | 23:DB:1740:G:C8   | 2.40                     | 0.57              |
| 23:DB:2256:G:O2'  | 43:DW:5:ALA:HB1   | 2.03                     | 0.57              |
| 26:DD:21:SER:C    | 26:DD:23:PRO:HD3  | 2.29                     | 0.57              |
| 26:DD:204:LYS:HE2 | 26:DD:204:LYS:HA  | 1.84                     | 0.57              |
| 45:DY:37:ARG:CZ   | 45:DY:37:ARG:HA   | 2.34                     | 0.57              |
| 46:DZ:47:LYS:HB2  | 46:DZ:51:VAL:CG1  | 2.34                     | 0.57              |
| 51:D4:11:CYS:HB2  | 51:D4:14:CYS:CB   | 2.28                     | 0.57              |
| 1:AA:335:C:H2'    | 1:AA:336:A:C8     | 2.39                     | 0.57              |
| 2:AC:77:GLY:HA3   | 2:AC:81:GLU:HB3   | 1.87                     | 0.57              |
| 8:AI:10:ARG:HB2   | 8:AI:14:SER:O     | 2.04                     | 0.57              |
| 9:AJ:15:HIS:HD2   | 9:AJ:18:ILE:HG22  | 1.69                     | 0.57              |
| 14:AO:57:ARG:HD3  | 14:AO:57:ARG:C    | 2.30                     | 0.57              |
| 23:BB:346:A:H2'   | 23:BB:347:A:O4'   | 2.04                     | 0.57              |
| 23:BB:404:A:H4'   | 23:BB:405:U:H5'   | 1.87                     | 0.57              |
| 23:BB:1560:G:H2'  | 23:BB:1561:C:H6   | 1.70                     | 0.57              |
| 23:BB:2352:A:H2'  | 23:BB:2353:G:O4'  | 2.04                     | 0.57              |
| 26:BD:2:ILE:HG12  | 26:BD:203:VAL:O   | 2.04                     | 0.57              |
| 27:BE:120:VAL:H   | 27:BE:189:THR:CG2 | 2.17                     | 0.57              |
| 27:BE:128:ALA:CB  | 27:BE:129:PRO:CD  | 2.81                     | 0.57              |
| 37:BP:25:VAL:HG23 | 37:BP:49:ILE:HD11 | 1.84                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 43:BW:49:ASN:HB2  | 43:BW:53:GLY:CA    | 2.34                     | 0.57              |
| 47:B0:52:LYS:HA   | 47:B0:52:LYS:HZ3   | 1.68                     | 0.57              |
| 50:B3:24:LYS:NZ   | 50:B3:29:ARG:HH22  | 2.02                     | 0.57              |
| 1:CA:114:U:O2'    | 1:CA:115:G:H5'     | 2.04                     | 0.57              |
| 1:CA:441:A:H61    | 1:CA:493:A:N6      | 2.02                     | 0.57              |
| 1:CA:552:U:H2'    | 1:CA:553:A:H8      | 1.70                     | 0.57              |
| 1:CA:1057:G:O3'   | 2:CC:196:GLY:HA3   | 2.04                     | 0.57              |
| 3:CD:115:GLN:NE2  | 3:CD:153:ARG:HH22  | 2.03                     | 0.57              |
| 4:CE:72:ASN:N     | 4:CE:72:ASN:HD22   | 2.01                     | 0.57              |
| 10:CK:12:ARG:HB3  | 10:CK:13:LYS:NZ    | 2.19                     | 0.57              |
| 18:CS:22:VAL:HG22 | 18:CS:42:ASN:OD1   | 2.04                     | 0.57              |
| 20:CB:209:VAL:C   | 20:CB:213:LEU:HD12 | 2.29                     | 0.57              |
| 23:DB:72:U:O2'    | 23:DB:73:A:H5'     | 2.04                     | 0.57              |
| 23:DB:182:A:H2'   | 23:DB:183:C:C6     | 2.39                     | 0.57              |
| 23:DB:230:G:H2'   | 23:DB:231:A:C8     | 2.39                     | 0.57              |
| 23:DB:301:G:H3'   | 23:DB:335:C:OP2    | 2.04                     | 0.57              |
| 23:DB:582:A:H2'   | 23:DB:583:G:H8     | 1.68                     | 0.57              |
| 23:DB:1082:U:C2   | 23:DB:1086:A:C6    | 2.92                     | 0.57              |
| 23:DB:2590:A:H2'  | 23:DB:2591:C:C6    | 2.40                     | 0.57              |
| 26:DD:22:ILE:HG23 | 26:DD:191:GLY:N    | 2.19                     | 0.57              |
| 26:DD:154:LYS:C   | 26:DD:156:PHE:H    | 2.12                     | 0.57              |
| 30:DH:26:ALA:HB3  | 30:DH:31:VAL:CG2   | 2.33                     | 0.57              |
| 32:DK:76:VAL:HB   | 37:DP:74:GLN:NE2   | 2.17                     | 0.57              |
| 36:DO:90:VAL:HG13 | 36:DO:116:GLN:H    | 1.68                     | 0.57              |
| 37:DP:25:VAL:HG12 | 37:DP:27:VAL:N     | 2.18                     | 0.57              |
| 41:DT:58:VAL:HG12 | 41:DT:59:ASN:H     | 1.69                     | 0.57              |
| 42:DU:38:ILE:HG13 | 42:DU:62:ALA:HB1   | 1.87                     | 0.57              |
| 44:DX:55:THR:HG22 | 44:DX:56:LEU:H     | 1.69                     | 0.57              |
| 45:DY:18:LYS:H    | 45:DY:18:LYS:CD    | 2.11                     | 0.57              |
| 46:DZ:55:GLY:HA2  | 46:DZ:59:ARG:HD2   | 1.86                     | 0.57              |
| 49:D2:12:ARG:HH21 | 49:D2:16:HIS:HB2   | 1.69                     | 0.57              |
| 1:AA:187:G:H4'    | 19:AT:79:THR:HG21  | 1.86                     | 0.57              |
| 1:AA:450:G:N7     | 1:AA:481:G:O6      | 2.37                     | 0.57              |
| 1:AA:950:U:H2'    | 1:AA:951:G:C8      | 2.39                     | 0.57              |
| 1:AA:1260:G:H4'   | 1:AA:1284:C:H5'    | 1.86                     | 0.57              |
| 1:AA:1508:A:H2'   | 1:AA:1509:C:H6     | 1.69                     | 0.57              |
| 3:AD:55:ARG:HH21  | 3:AD:58:GLN:NE2    | 2.02                     | 0.57              |
| 6:AG:14:ASP:OD2   | 6:AG:22:LEU:HD12   | 2.04                     | 0.57              |
| 8:AI:51:LEU:HD23  | 8:AI:56:MET:CE     | 2.31                     | 0.57              |
| 22:BA:50:A:H5''   | 36:BO:68:LYS:CD    | 2.33                     | 0.57              |
| 23:BB:15:G:O2'    | 23:BB:16:C:H5'     | 2.05                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BB:727:A:OP1   | 23:BB:1431:A:O2'  | 2.21                     | 0.57              |
| 23:BB:2307:G:H4'  | 23:BB:2311:A:H61  | 1.68                     | 0.57              |
| 24:BV:80:HIS:N    | 24:BV:87:GLN:HE22 | 2.02                     | 0.57              |
| 26:BD:2:ILE:HB    | 26:BD:205:PRO:HD3 | 1.85                     | 0.57              |
| 29:BG:84:LYS:HZ2  | 29:BG:85:LYS:H    | 1.50                     | 0.57              |
| 31:BJ:25:LEU:N    | 31:BJ:25:LEU:HD13 | 2.19                     | 0.57              |
| 34:BM:108:VAL:N   | 34:BM:109:PRO:HD3 | 2.19                     | 0.57              |
| 35:BN:10:LEU:H    | 35:BN:17:ARG:NH1  | 2.02                     | 0.57              |
| 35:BN:29:VAL:HG21 | 35:BN:75:ILE:HD11 | 1.86                     | 0.57              |
| 36:BO:40:ILE:H    | 36:BO:40:ILE:HD13 | 1.69                     | 0.57              |
| 40:BS:18:ARG:NH1  | 40:BS:25:ARG:HH22 | 2.02                     | 0.57              |
| 41:BT:10:VAL:O    | 41:BT:34:VAL:HG13 | 2.05                     | 0.57              |
| 1:CA:265:G:H2'    | 1:CA:267:C:H5     | 1.69                     | 0.57              |
| 1:CA:383:A:H2'    | 1:CA:384:G:O4'    | 2.05                     | 0.57              |
| 1:CA:411:A:C4     | 1:CA:413:G:H1'    | 2.40                     | 0.57              |
| 1:CA:1105:A:H2'   | 1:CA:1106:G:H8    | 1.69                     | 0.57              |
| 1:CA:1461:G:H2'   | 1:CA:1462:C:C6    | 2.39                     | 0.57              |
| 4:CE:73:VAL:HG21  | 4:CE:143:LEU:O    | 2.04                     | 0.57              |
| 14:CO:53:ARG:HH11 | 14:CO:53:ARG:HG2  | 1.68                     | 0.57              |
| 23:DB:196:A:H2'   | 23:DB:196:A:N3    | 2.19                     | 0.57              |
| 23:DB:536:G:H5''  | 38:DQ:52:ARG:NH2  | 2.20                     | 0.57              |
| 23:DB:849:A:H2'   | 23:DB:850:U:C6    | 2.40                     | 0.57              |
| 23:DB:877:A:H2    | 23:DB:900:A:N7    | 2.02                     | 0.57              |
| 23:DB:1932:A:H2'  | 23:DB:1933:G:O4'  | 2.04                     | 0.57              |
| 23:DB:2053:G:H5'  | 26:DD:149:ASN:O   | 2.04                     | 0.57              |
| 23:DB:2283:C:H5'' | 23:DB:2389:G:O2'  | 2.04                     | 0.57              |
| 23:DB:2376:A:N3   | 36:DO:111:ARG:NH2 | 2.52                     | 0.57              |
| 23:DB:2617:U:C2'  | 23:DB:2618:G:H5'  | 2.35                     | 0.57              |
| 23:DB:2819:G:H2'  | 23:DB:2821:A:N7   | 2.19                     | 0.57              |
| 30:DH:113:SER:HB2 | 30:DH:132:PHE:HZ  | 1.69                     | 0.57              |
| 33:DL:30:THR:HG21 | 33:DL:38:GLN:NE2  | 2.20                     | 0.57              |
| 39:DR:80:ARG:CZ   | 39:DR:85:LYS:HB3  | 2.34                     | 0.57              |
| 51:D4:16:ILE:HG23 | 51:D4:18:LYS:H    | 1.69                     | 0.57              |
| 52:DI:27:LEU:HD23 | 52:DI:27:LEU:N    | 2.15                     | 0.57              |
| 1:AA:1320:C:H41   | 18:AS:36:ARG:CG   | 2.18                     | 0.57              |
| 1:AA:1366:C:H2'   | 1:AA:1367:C:C6    | 2.39                     | 0.57              |
| 13:AN:66:THR:HG23 | 13:AN:67:GLY:H    | 1.69                     | 0.57              |
| 23:BB:264:C:O2'   | 23:BB:265:A:H5''  | 2.05                     | 0.57              |
| 23:BB:285:G:O2'   | 23:BB:286:U:H5'   | 2.05                     | 0.57              |
| 23:BB:716:A:H2'   | 23:BB:717:C:O4'   | 2.03                     | 0.57              |
| 23:BB:918:A:C2'   | 23:BB:919:U:H5'   | 2.34                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:BB:1438:U:N3    | 23:BB:1552:A:N6   | 2.53                     | 0.57              |
| 23:BB:1505:A:H2'   | 23:BB:1506:U:C6   | 2.39                     | 0.57              |
| 23:BB:1537:G:H2'   | 23:BB:1538:G:C4'  | 2.35                     | 0.57              |
| 23:BB:1878:G:H2'   | 23:BB:1879:C:H6   | 1.69                     | 0.57              |
| 24:BV:84:PRO:HG3   | 34:BM:127:LYS:NZ  | 2.19                     | 0.57              |
| 25:BC:76:VAL:O     | 25:BC:93:VAL:HA   | 2.04                     | 0.57              |
| 27:BE:48:THR:HG22  | 27:BE:49:ARG:N    | 2.14                     | 0.57              |
| 27:BE:108:ILE:HG21 | 27:BE:116:ASP:OD2 | 2.04                     | 0.57              |
| 27:BE:116:ASP:O    | 27:BE:117:ARG:HB3 | 2.05                     | 0.57              |
| 28:BF:177:ARG:HE   | 28:BF:178:LYS:CA  | 2.17                     | 0.57              |
| 31:BJ:25:LEU:HG    | 31:BJ:63:ALA:H    | 1.69                     | 0.57              |
| 34:BM:34:LYS:HD3   | 34:BM:98:PRO:O    | 2.04                     | 0.57              |
| 36:BO:17:LYS:HE3   | 36:BO:43:ASN:HB2  | 1.86                     | 0.57              |
| 42:BU:78:LYS:HG3   | 42:BU:96:LYS:HE3  | 1.85                     | 0.57              |
| 43:BW:49:ASN:HD22  | 43:BW:53:GLY:HA2  | 1.68                     | 0.57              |
| 48:B1:15:GLY:N     | 48:B1:47:ILE:HD12 | 2.19                     | 0.57              |
| 1:CA:238:A:C2'     | 1:CA:239:U:H5''   | 2.31                     | 0.57              |
| 1:CA:972:C:OP1     | 9:CJ:59:LYS:HD2   | 2.04                     | 0.57              |
| 3:CD:58:GLN:O      | 3:CD:62:ARG:HG2   | 2.04                     | 0.57              |
| 9:CJ:36:VAL:HA     | 9:CJ:76:ILE:HG23  | 1.87                     | 0.57              |
| 9:CJ:37:ARG:HH11   | 9:CJ:37:ARG:HG2   | 1.68                     | 0.57              |
| 12:CM:48:SER:H     | 12:CM:51:GLN:NE2  | 2.03                     | 0.57              |
| 20:CB:104:LYS:HB2  | 20:CB:104:LYS:NZ  | 2.20                     | 0.57              |
| 20:CB:169:HIS:CE1  | 20:CB:173:LYS:HB2 | 2.40                     | 0.57              |
| 21:CU:41:THR:CA    | 21:CU:45:LYS:HD3  | 2.32                     | 0.57              |
| 22:DA:59:A:H2'     | 22:DA:60:C:O4'    | 2.05                     | 0.57              |
| 23:DB:1637:A:H2'   | 23:DB:1638:C:C6   | 2.39                     | 0.57              |
| 23:DB:1791:A:H5''  | 25:DC:211:ARG:HE  | 1.70                     | 0.57              |
| 23:DB:2085:U:O2'   | 23:DB:2086:U:H5'  | 2.05                     | 0.57              |
| 23:DB:2329:U:H2'   | 23:DB:2330:G:H8   | 1.69                     | 0.57              |
| 23:DB:2869:G:H2'   | 23:DB:2870:C:C6   | 2.40                     | 0.57              |
| 24:DV:4:ILE:HD12   | 24:DV:4:ILE:N     | 2.19                     | 0.57              |
| 33:DL:39:LYS:HA    | 33:DL:39:LYS:HZ2  | 1.70                     | 0.57              |
| 33:DL:81:ASP:HA    | 33:DL:84:LYS:HB3  | 1.86                     | 0.57              |
| 34:DM:5:LYS:HA     | 34:DM:68:PHE:CE1  | 2.40                     | 0.57              |
| 36:DO:18:LEU:HD21  | 36:DO:43:ASN:ND2  | 2.19                     | 0.57              |
| 37:DP:47:ILE:CG2   | 37:DP:48:ALA:H    | 2.03                     | 0.57              |
| 42:DU:12:VAL:HG11  | 42:DU:17:ASP:HB3  | 1.87                     | 0.57              |
| 51:D4:26:ILE:O     | 51:D4:27:CYS:CB   | 2.52                     | 0.57              |
| 52:DI:37:PHE:CZ    | 52:DI:58:ILE:HD11 | 2.39                     | 0.57              |
| 52:DI:45:THR:HA    | 52:DI:48:ILE:CG2  | 2.33                     | 0.57              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:71:A:N1       | 1:AA:99:C:H1'      | 2.19                     | 0.57              |
| 1:AA:202:G:H2'     | 1:AA:203:G:H8      | 1.70                     | 0.57              |
| 1:AA:411:A:C4      | 1:AA:413:G:H1'     | 2.40                     | 0.57              |
| 1:AA:1283:U:H2'    | 1:AA:1284:C:C6     | 2.40                     | 0.57              |
| 4:AE:81:GLN:HE22   | 4:AE:82:HIS:CE1    | 2.23                     | 0.57              |
| 6:AG:14:ASP:H      | 6:AG:19:SER:H      | 1.51                     | 0.57              |
| 16:AQ:7:LEU:HD13   | 16:AQ:24:ILE:HG12  | 1.87                     | 0.57              |
| 18:AS:11:ASP:H     | 18:AS:37:SER:HB3   | 1.68                     | 0.57              |
| 21:AU:39:LYS:N     | 21:AU:40:PRO:CD    | 2.66                     | 0.57              |
| 23:BB:548:G:H5'    | 23:BB:549:G:O4'    | 2.03                     | 0.57              |
| 23:BB:871:U:H2'    | 23:BB:872:U:H6     | 1.68                     | 0.57              |
| 23:BB:1131:G:C1'   | 31:BJ:85:LYS:HZ2   | 2.18                     | 0.57              |
| 23:BB:1180:U:O2'   | 23:BB:1181:U:H5'   | 2.05                     | 0.57              |
| 23:BB:1637:A:H2'   | 23:BB:1638:C:C6    | 2.40                     | 0.57              |
| 23:BB:2083:G:H2'   | 23:BB:2084:C:H6    | 1.69                     | 0.57              |
| 27:BE:112:LEU:HB3  | 27:BE:116:ASP:H    | 1.69                     | 0.57              |
| 33:BL:78:ARG:NH1   | 33:BL:110:VAL:HG11 | 2.20                     | 0.57              |
| 33:BL:79:LEU:HB3   | 33:BL:114:GLY:N    | 2.12                     | 0.57              |
| 34:BM:96:ILE:HD13  | 34:BM:97:GLN:CG    | 2.34                     | 0.57              |
| 37:BP:62:LYS:HD3   | 37:BP:72:VAL:HG21  | 1.87                     | 0.57              |
| 38:BQ:51:GLN:O     | 38:BQ:54:ARG:HG2   | 2.05                     | 0.57              |
| 51:B4:22:VAL:HG11  | 51:B4:36:ARG:NH1   | 2.20                     | 0.57              |
| 22:DA:113:C:O2'    | 36:DO:47:VAL:HA    | 2.04                     | 0.57              |
| 23:DB:453:A:H4'    | 23:DB:472:A:H61    | 1.69                     | 0.57              |
| 23:DB:1309:G:C4'   | 49:D2:7:PRO:HB2    | 2.34                     | 0.57              |
| 23:DB:1441:G:H2'   | 23:DB:1442:U:C6    | 2.40                     | 0.57              |
| 23:DB:1464:G:H2'   | 23:DB:1465:G:H8    | 1.68                     | 0.57              |
| 23:DB:1505:A:H2'   | 23:DB:1506:U:C6    | 2.39                     | 0.57              |
| 23:DB:2105:U:H2'   | 23:DB:2106:U:H6    | 1.68                     | 0.57              |
| 23:DB:2480:C:O2'   | 23:DB:2481:G:H5'   | 2.03                     | 0.57              |
| 23:DB:2722:G:O2'   | 35:DN:4:ARG:NE     | 2.38                     | 0.57              |
| 25:DC:156:SER:O    | 25:DC:195:GLY:HA3  | 2.05                     | 0.57              |
| 25:DC:179:GLU:CG   | 25:DC:266:ILE:HA   | 2.34                     | 0.57              |
| 26:DD:122:VAL:CA   | 26:DD:128:ARG:HG3  | 2.33                     | 0.57              |
| 27:DE:133:LEU:HD22 | 27:DE:136:GLN:HG3  | 1.87                     | 0.57              |
| 28:DF:120:SER:HB3  | 28:DF:127:TYR:CE1  | 2.40                     | 0.57              |
| 29:DG:124:CYS:HB3  | 29:DG:130:ILE:HD13 | 1.87                     | 0.57              |
| 30:DH:6:LEU:HB2    | 30:DH:35:LYS:HB2   | 1.85                     | 0.57              |
| 30:DH:96:THR:HG23  | 30:DH:97:ARG:H     | 1.68                     | 0.57              |
| 32:DK:70:ARG:CD    | 32:DK:76:VAL:HG22  | 2.33                     | 0.57              |
| 33:DL:133:ALA:O    | 33:DL:136:GLU:HB2  | 2.04                     | 0.57              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:DM:33:LEU:HD22 | 34:DM:124:LEU:HD22 | 1.85                     | 0.57              |
| 36:DO:15:ARG:HH22 | 43:DW:76:ARG:CD    | 2.16                     | 0.57              |
| 37:DP:1:SER:HA    | 37:DP:4:ILE:HB     | 1.86                     | 0.57              |
| 37:DP:27:VAL:HA   | 37:DP:86:LYS:CE    | 2.32                     | 0.57              |
| 38:DQ:65:ASN:HB2  | 38:DQ:75:TYR:HB2   | 1.87                     | 0.57              |
| 38:DQ:111:LYS:NZ  | 39:DR:52:PRO:HA    | 2.20                     | 0.57              |
| 40:DS:87:PRO:O    | 40:DS:93:ALA:HA    | 2.05                     | 0.57              |
| 52:DI:100:ILE:O   | 52:DI:139:VAL:HA   | 2.04                     | 0.57              |
| 1:AA:85:U:H4'     | 1:AA:86:G:H4'      | 1.85                     | 0.57              |
| 1:AA:114:U:O2'    | 1:AA:115:G:H5'     | 2.04                     | 0.57              |
| 1:AA:413:G:H4'    | 1:AA:414:A:H5''    | 1.85                     | 0.57              |
| 1:AA:973:G:H3'    | 1:AA:974:A:H5''    | 1.87                     | 0.57              |
| 1:AA:1179:A:H4'   | 8:AI:104:THR:HA    | 1.86                     | 0.57              |
| 1:AA:1376:U:H2'   | 1:AA:1377:A:H8     | 1.69                     | 0.57              |
| 2:AC:21:TRP:HB3   | 2:AC:58:ARG:HB2    | 1.86                     | 0.57              |
| 2:AC:76:ILE:C     | 2:AC:82:ASP:HB2    | 2.30                     | 0.57              |
| 3:AD:25:ARG:HH11  | 3:AD:30:LYS:HE3    | 1.69                     | 0.57              |
| 6:AG:16:LYS:HD3   | 6:AG:16:LYS:C      | 2.29                     | 0.57              |
| 8:AI:107:ALA:O    | 8:AI:109:GLN:HG2   | 2.05                     | 0.57              |
| 10:AK:95:THR:HG23 | 10:AK:96:ILE:N     | 2.19                     | 0.57              |
| 11:AL:34:THR:HB   | 11:AL:53:ARG:HB2   | 1.87                     | 0.57              |
| 20:AB:102:ASN:O   | 20:AB:106:VAL:HG23 | 2.04                     | 0.57              |
| 21:AU:11:PHE:HD1  | 21:AU:11:PHE:O     | 1.86                     | 0.57              |
| 23:BB:519:U:H5''  | 40:BS:18:ARG:NH2   | 2.20                     | 0.57              |
| 23:BB:632:A:H2'   | 23:BB:633:A:C8     | 2.40                     | 0.57              |
| 23:BB:1220:G:H2'  | 23:BB:1221:C:C6    | 2.40                     | 0.57              |
| 23:BB:2650:U:H2'  | 23:BB:2651:C:H6    | 1.69                     | 0.57              |
| 23:BB:2819:G:H2'  | 23:BB:2821:A:N7    | 2.19                     | 0.57              |
| 23:BB:2872:A:O2'  | 23:BB:2873:A:H5''  | 2.05                     | 0.57              |
| 23:BB:2882:A:H2'  | 23:BB:2883:A:H5''  | 1.86                     | 0.57              |
| 24:BV:44:HIS:NE2  | 24:BV:85:LYS:HB2   | 2.19                     | 0.57              |
| 28:BF:68:LYS:HA   | 28:BF:83:PRO:HA    | 1.86                     | 0.57              |
| 31:BJ:56:VAL:C    | 31:BJ:57:LEU:HD22  | 2.29                     | 0.57              |
| 32:BK:53:LYS:HE2  | 32:BK:56:ASP:OD1   | 2.04                     | 0.57              |
| 40:BS:6:LYS:HA    | 40:BS:104:THR:CA   | 2.28                     | 0.57              |
| 41:BT:64:LYS:HB3  | 41:BT:77:ARG:HD3   | 1.87                     | 0.57              |
| 43:BW:36:ILE:HG22 | 43:BW:36:ILE:O     | 2.05                     | 0.57              |
| 46:BZ:50:ASP:HA   | 46:BZ:53:THR:HG22  | 1.86                     | 0.57              |
| 51:B4:33:HIS:H    | 51:B4:33:HIS:HD2   | 1.51                     | 0.57              |
| 1:CA:384:G:H2'    | 1:CA:385:C:H6      | 1.68                     | 0.57              |
| 1:CA:1175:G:O2'   | 1:CA:1176:A:H5'    | 2.04                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:CE:142:GLY:HA2  | 4:CE:145:ASN:HD22  | 1.70                     | 0.57              |
| 5:CF:38:ARG:NH2   | 5:CF:96:VAL:HB     | 2.20                     | 0.57              |
| 7:CH:101:ALA:O    | 7:CH:103:VAL:HG23  | 2.04                     | 0.57              |
| 13:CN:40:ARG:HG3  | 18:CS:6:LYS:O      | 2.05                     | 0.57              |
| 22:DA:112:G:O2'   | 22:DA:113:C:H5'    | 2.04                     | 0.57              |
| 23:DB:558:U:P     | 31:DJ:113:PRO:HB2  | 2.45                     | 0.57              |
| 23:DB:1381:G:O2'  | 23:DB:1382:G:H5'   | 2.05                     | 0.57              |
| 23:DB:1400:U:H2'  | 23:DB:1401:G:H8    | 1.70                     | 0.57              |
| 23:DB:1722:A:H61  | 23:DB:1738:G:H1'   | 1.69                     | 0.57              |
| 23:DB:1729:U:H2'  | 23:DB:1730:C:H4'   | 1.87                     | 0.57              |
| 23:DB:1842:G:H2'  | 23:DB:1843:C:H6    | 1.70                     | 0.57              |
| 23:DB:2352:A:H2'  | 23:DB:2353:G:O4'   | 2.04                     | 0.57              |
| 23:DB:2455:G:H2'  | 23:DB:2456:C:H6    | 1.70                     | 0.57              |
| 24:DV:82:TYR:HE1  | 24:DV:83:LYS:HE3   | 1.70                     | 0.57              |
| 25:DC:53:ILE:HD13 | 25:DC:218:THR:HG23 | 1.87                     | 0.57              |
| 27:DE:99:LYS:HZ2  | 27:DE:100:MET:N    | 2.02                     | 0.57              |
| 27:DE:109:LEU:HG  | 27:DE:117:ARG:CD   | 2.34                     | 0.57              |
| 29:DG:163:TYR:HB2 | 29:DG:166:GLU:HG3  | 1.85                     | 0.57              |
| 31:DJ:89:PHE:HD1  | 31:DJ:92:MET:HG3   | 1.68                     | 0.57              |
| 33:DL:109:LYS:HA  | 33:DL:127:VAL:H    | 1.69                     | 0.57              |
| 35:DN:35:LYS:HE3  | 35:DN:110:MET:HB3  | 1.86                     | 0.57              |
| 36:DO:83:LEU:HA   | 36:DO:87:ILE:HD12  | 1.87                     | 0.57              |
| 41:DT:3:ARG:HB3   | 41:DT:5:GLU:OE2    | 2.04                     | 0.57              |
| 43:DW:42:THR:HG23 | 43:DW:66:VAL:N     | 2.18                     | 0.57              |
| 44:DX:17:GLU:HA   | 44:DX:21:LEU:HB2   | 1.85                     | 0.57              |
| 45:DY:10:ARG:O    | 45:DY:11:SER:HB3   | 2.04                     | 0.57              |
| 1:AA:537:G:H5''   | 11:AL:109:ARG:HH11 | 1.69                     | 0.57              |
| 1:AA:1081:A:O2'   | 1:AA:1082:A:H5'    | 2.05                     | 0.57              |
| 1:AA:1101:A:H61   | 20:AB:173:LYS:HD2  | 1.70                     | 0.57              |
| 2:AC:110:LEU:HB3  | 2:AC:203:LYS:HZ3   | 1.70                     | 0.57              |
| 5:AF:3:HIS:HB2    | 5:AF:92:THR:CB     | 2.35                     | 0.57              |
| 8:AI:113:LYS:HA   | 8:AI:120:ALA:HB2   | 1.87                     | 0.57              |
| 9:AJ:42:LEU:HB2   | 9:AJ:71:LEU:HD13   | 1.85                     | 0.57              |
| 23:BB:127:A:H5''  | 23:BB:128:C:C6     | 2.40                     | 0.57              |
| 23:BB:643:A:H61   | 23:BB:2370:G:H1'   | 1.68                     | 0.57              |
| 23:BB:2270:A:H4'  | 43:BW:18:LYS:CB    | 2.35                     | 0.57              |
| 23:BB:2455:G:H2'  | 23:BB:2456:C:H6    | 1.70                     | 0.57              |
| 25:BC:154:ALA:C   | 25:BC:156:SER:H    | 2.13                     | 0.57              |
| 28:BF:44:ALA:HB1  | 28:BF:48:LEU:HD12  | 1.86                     | 0.57              |
| 36:BO:17:LYS:HE2  | 43:BW:77:LYS:CD    | 2.35                     | 0.57              |
| 38:BQ:32:ARG:O    | 38:BQ:36:GLN:HB2   | 2.05                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:BU:11:ILE:HB    | 42:BU:69:VAL:CB    | 2.35                     | 0.57              |
| 42:BU:52:ASN:C     | 42:BU:54:PRO:HD3   | 2.30                     | 0.57              |
| 1:CA:1414:U:H2'    | 1:CA:1415:G:H8     | 1.69                     | 0.57              |
| 23:DB:165:A:H2'    | 23:DB:166:U:H6     | 1.69                     | 0.57              |
| 23:DB:170:U:H2'    | 23:DB:171:U:C6     | 2.39                     | 0.57              |
| 23:DB:506:G:H4'    | 23:DB:509:C:O2     | 2.05                     | 0.57              |
| 23:DB:1100:C:OP2   | 52:DI:2:LYS:HB3    | 2.05                     | 0.57              |
| 23:DB:1198:U:H2'   | 23:DB:1199:U:H6    | 1.70                     | 0.57              |
| 23:DB:1198:U:H2'   | 23:DB:1199:U:C6    | 2.39                     | 0.57              |
| 23:DB:1946:U:H2'   | 23:DB:1947:C:H6    | 1.69                     | 0.57              |
| 23:DB:2378:A:H2'   | 23:DB:2379:G:H5'   | 1.85                     | 0.57              |
| 23:DB:2902:C:O2'   | 23:DB:2903:U:H4'   | 2.05                     | 0.57              |
| 25:DC:22:GLU:CD    | 25:DC:202:ARG:HE   | 2.12                     | 0.57              |
| 25:DC:62:ARG:O     | 25:DC:63:ILE:HB    | 2.05                     | 0.57              |
| 28:DF:36:ASN:HB2   | 28:DF:87:LYS:HA    | 1.87                     | 0.57              |
| 38:DQ:48:ASP:CA    | 38:DQ:51:GLN:HE21  | 2.06                     | 0.57              |
| 43:DW:24:ARG:HB3   | 43:DW:59:PHE:CD2   | 2.39                     | 0.57              |
| 51:D4:24:ARG:HH21  | 51:D4:37:GLN:HB2   | 1.69                     | 0.57              |
| 52:DI:32:VAL:HG22  | 52:DI:60:VAL:CG2   | 2.34                     | 0.57              |
| 1:AA:212:G:H2'     | 1:AA:213:G:H8      | 1.68                     | 0.57              |
| 2:AC:33:ASP:OD2    | 13:AN:64:ARG:HD3   | 2.05                     | 0.57              |
| 7:AH:29:SER:HB3    | 7:AH:32:LYS:CG     | 2.35                     | 0.57              |
| 10:AK:126:ARG:HB2  | 21:AU:33:ARG:CD    | 2.30                     | 0.57              |
| 15:AP:25:ARG:HD3   | 15:AP:25:ARG:N     | 2.20                     | 0.57              |
| 18:AS:28:LYS:HB2   | 18:AS:29:PRO:HD2   | 1.87                     | 0.57              |
| 20:AB:37:VAL:HG22  | 20:AB:38:HIS:H     | 1.68                     | 0.57              |
| 20:AB:71:THR:CG2   | 20:AB:94:ARG:HH21  | 2.18                     | 0.57              |
| 23:BB:49:A:OP1     | 23:BB:51:G:H5'     | 2.05                     | 0.57              |
| 23:BB:459:U:C5'    | 49:B2:41:ARG:HE    | 2.16                     | 0.57              |
| 23:BB:1400:U:H2'   | 23:BB:1401:G:H8    | 1.70                     | 0.57              |
| 23:BB:2213:U:C2'   | 23:BB:2213:U:O2    | 2.52                     | 0.57              |
| 23:BB:2567:G:H2'   | 23:BB:2568:U:C6    | 2.40                     | 0.57              |
| 23:BB:2839:G:H2'   | 23:BB:2840:C:H6    | 1.70                     | 0.57              |
| 24:BV:61:LEU:O     | 24:BV:71:LYS:HA    | 2.05                     | 0.57              |
| 25:BC:143:VAL:HG12 | 25:BC:144:GLU:N    | 2.14                     | 0.57              |
| 25:BC:224:MET:HG3  | 25:BC:233:GLY:O    | 2.05                     | 0.57              |
| 26:BD:193:VAL:O    | 26:BD:193:VAL:HG13 | 2.03                     | 0.57              |
| 32:BK:70:ARG:CB    | 32:BK:76:VAL:HG22  | 2.31                     | 0.57              |
| 33:BL:129:LYS:HD3  | 33:BL:129:LYS:O    | 2.05                     | 0.57              |
| 35:BN:22:ARG:HG3   | 35:BN:23:ASN:N     | 2.17                     | 0.57              |
| 37:BP:55:HIS:O     | 37:BP:57:ALA:N     | 2.38                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:BP:62:LYS:HE3   | 37:BP:74:GLN:NE2   | 2.19                     | 0.57              |
| 38:BQ:50:ARG:HG3   | 38:BQ:53:LYS:NZ    | 2.20                     | 0.57              |
| 38:BQ:85:ALA:HB1   | 38:BQ:88:GLU:HB2   | 1.87                     | 0.57              |
| 39:BR:41:ILE:C     | 39:BR:43:ASN:N     | 2.60                     | 0.57              |
| 39:BR:49:ILE:HG22  | 39:BR:51:VAL:HG23  | 1.86                     | 0.57              |
| 39:BR:58:VAL:HG22  | 39:BR:59:ILE:N     | 2.17                     | 0.57              |
| 39:BR:77:PHE:C     | 39:BR:78:ARG:HG3   | 2.30                     | 0.57              |
| 40:BS:1:MET:HB3    | 40:BS:4:ILE:HG12   | 1.86                     | 0.57              |
| 41:BT:12:ARG:NH2   | 44:BX:29:ARG:HH12  | 2.01                     | 0.57              |
| 42:BU:2:ALA:O      | 42:BU:4:ILE:N      | 2.37                     | 0.57              |
| 42:BU:9:GLU:HA     | 42:BU:23:LYS:HA    | 1.86                     | 0.57              |
| 42:BU:79:ALA:O     | 42:BU:96:LYS:HA    | 2.04                     | 0.57              |
| 44:BX:29:ARG:N     | 44:BX:34:SER:HB2   | 2.19                     | 0.57              |
| 1:CA:619:U:H3      | 3:CD:130:ASN:HD21  | 1.53                     | 0.57              |
| 1:CA:908:A:H2'     | 1:CA:909:A:H8      | 1.70                     | 0.57              |
| 1:CA:1134:G:C6     | 1:CA:1135:U:H1'    | 2.40                     | 0.57              |
| 2:CC:115:VAL:O     | 2:CC:119:ILE:HG22  | 2.05                     | 0.57              |
| 2:CC:143:LEU:H     | 2:CC:143:LEU:HD13  | 1.70                     | 0.57              |
| 8:CI:93:LEU:O      | 8:CI:97:LEU:HG     | 2.05                     | 0.57              |
| 21:CU:34:ARG:HG2   | 21:CU:35:GLU:N     | 2.10                     | 0.57              |
| 23:DB:125:A:H4'    | 23:DB:126:A:OP2    | 2.05                     | 0.57              |
| 23:DB:544:C:O2'    | 23:DB:545:U:O5'    | 2.23                     | 0.57              |
| 23:DB:546:U:H5'    | 23:DB:546:U:O2     | 2.05                     | 0.57              |
| 23:DB:765:C:H2'    | 23:DB:766:U:C6     | 2.40                     | 0.57              |
| 23:DB:962:G:N2     | 34:DM:81:ARG:HD3   | 2.20                     | 0.57              |
| 23:DB:1211:C:H4'   | 23:DB:1212:G:OP2   | 2.04                     | 0.57              |
| 23:DB:1537:G:H2'   | 23:DB:1538:G:C4'   | 2.35                     | 0.57              |
| 23:DB:1791:A:C2    | 23:DB:1829:A:C4'   | 2.88                     | 0.57              |
| 23:DB:1853:A:N1    | 23:DB:2087:G:H1'   | 2.19                     | 0.57              |
| 23:DB:2234:G:O2'   | 23:DB:2235:G:H5'   | 2.04                     | 0.57              |
| 25:DC:237:ARG:HH11 | 25:DC:238:ASN:HA   | 1.69                     | 0.57              |
| 28:DF:106:ALA:HB1  | 28:DF:136:ILE:HG22 | 1.85                     | 0.57              |
| 32:DK:6:THR:O      | 32:DK:20:MET:HG3   | 2.05                     | 0.57              |
| 32:DK:24:VAL:HA    | 32:DK:39:ILE:HD12  | 1.86                     | 0.57              |
| 37:DP:6:GLN:CD     | 37:DP:6:GLN:N      | 2.63                     | 0.57              |
| 38:DQ:69:ARG:HH11  | 38:DQ:69:ARG:CB    | 2.16                     | 0.57              |
| 45:DY:8:GLN:HB2    | 45:DY:28:LEU:HG    | 1.87                     | 0.57              |
| 1:AA:265:G:H2'     | 1:AA:267:C:H5      | 1.69                     | 0.57              |
| 1:AA:600:A:OP1     | 7:AH:88:LYS:HG2    | 2.04                     | 0.57              |
| 1:AA:784:A:H2'     | 1:AA:785:G:H8      | 1.70                     | 0.57              |
| 1:AA:993:G:H4'     | 1:AA:994:A:OP2     | 2.05                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1225:A:H4'    | 18:AS:77:ARG:NH2   | 2.20                     | 0.57              |
| 2:AC:46:LEU:HD23   | 2:AC:75:VAL:HG13   | 1.86                     | 0.57              |
| 3:AD:117:VAL:HG12  | 3:AD:130:ASN:C     | 2.30                     | 0.57              |
| 3:AD:170:LEU:HD12  | 3:AD:170:LEU:O     | 2.05                     | 0.57              |
| 4:AE:155:LYS:HA    | 7:AH:65:PHE:CD1    | 2.40                     | 0.57              |
| 8:AI:11:ARG:NH2    | 8:AI:12:LYS:HE3    | 2.20                     | 0.57              |
| 8:AI:44:ARG:HH11   | 8:AI:44:ARG:N      | 2.02                     | 0.57              |
| 12:AM:21:ILE:HB    | 12:AM:24:VAL:HG22  | 1.87                     | 0.57              |
| 13:AN:17:ASP:HA    | 13:AN:21:ALA:HB2   | 1.87                     | 0.57              |
| 20:AB:165:ALA:HB2  | 20:AB:186:VAL:HG12 | 1.87                     | 0.57              |
| 23:BB:182:A:H2'    | 23:BB:183:C:H6     | 1.70                     | 0.57              |
| 23:BB:278:A:N3     | 23:BB:278:A:H2'    | 2.20                     | 0.57              |
| 23:BB:609:A:H2'    | 23:BB:610:C:O4'    | 2.05                     | 0.57              |
| 23:BB:702:U:O2'    | 23:BB:703:U:H5'    | 2.05                     | 0.57              |
| 23:BB:1155:A:OP1   | 38:BQ:54:ARG:HD2   | 2.05                     | 0.57              |
| 23:BB:1790:C:H4'   | 25:BC:207:ALA:HB2  | 1.86                     | 0.57              |
| 23:BB:2371:G:O2'   | 48:B1:44:GLN:HA    | 2.04                     | 0.57              |
| 23:BB:2617:U:C2'   | 23:BB:2618:G:H5'   | 2.35                     | 0.57              |
| 28:BF:18:GLU:C     | 28:BF:20:ASN:H     | 2.12                     | 0.57              |
| 36:BO:43:ASN:HA    | 36:BO:46:GLU:OE2   | 2.04                     | 0.57              |
| 36:BO:60:GLU:HG3   | 36:BO:61:GLN:H     | 1.70                     | 0.57              |
| 42:BU:81:ARG:N     | 42:BU:81:ARG:HD2   | 2.19                     | 0.57              |
| 43:BW:16:GLU:HG2   | 43:BW:37:VAL:HG22  | 1.85                     | 0.57              |
| 47:B0:24:VAL:O     | 47:B0:25:THR:HG23  | 2.05                     | 0.57              |
| 49:B2:30:VAL:HA    | 49:B2:33:ARG:HD2   | 1.87                     | 0.57              |
| 1:CA:51:A:O2'      | 1:CA:52:C:OP2      | 2.18                     | 0.57              |
| 1:CA:674:G:H2'     | 1:CA:675:A:C8      | 2.40                     | 0.57              |
| 8:CI:56:MET:SD     | 8:CI:57:VAL:N      | 2.78                     | 0.57              |
| 9:CJ:52:LEU:HG     | 9:CJ:62:ARG:HE     | 1.70                     | 0.57              |
| 23:DB:632:A:H2'    | 23:DB:633:A:C8     | 2.40                     | 0.57              |
| 23:DB:796:C:H2'    | 23:DB:797:G:C8     | 2.40                     | 0.57              |
| 23:DB:997:G:C5'    | 38:DQ:92:LYS:HG3   | 2.35                     | 0.57              |
| 23:DB:2339:C:H2'   | 23:DB:2340:A:H8    | 1.68                     | 0.57              |
| 23:DB:2820:A:C6    | 26:DD:197:THR:HB   | 2.40                     | 0.57              |
| 24:DV:44:HIS:C     | 24:DV:46:LYS:H     | 2.13                     | 0.57              |
| 25:DC:163:ILE:HG12 | 25:DC:173:LEU:HD21 | 1.87                     | 0.57              |
| 27:DE:91:ASP:O     | 27:DE:92:HIS:HB2   | 2.05                     | 0.57              |
| 33:DL:55:MET:CB    | 33:DL:56:PRO:HD3   | 2.35                     | 0.57              |
| 35:DN:73:ASN:HA    | 35:DN:76:VAL:CG1   | 2.35                     | 0.57              |
| 51:D4:11:CYS:SG    | 51:D4:26:ILE:C     | 2.88                     | 0.57              |
| 52:DI:23:VAL:HG12  | 52:DI:27:LEU:HD21  | 1.87                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:441:A:H61    | 1:AA:493:A:N6      | 2.03                     | 0.56              |
| 1:AA:1074:G:H5'   | 20:AB:104:LYS:NZ   | 2.19                     | 0.56              |
| 1:AA:1342:C:H5'   | 8:AI:127:SER:HA    | 1.86                     | 0.56              |
| 4:AE:92:ARG:HB3   | 4:AE:127:TYR:HB2   | 1.87                     | 0.56              |
| 6:AG:139:ASP:HA   | 6:AG:142:ARG:HH12  | 1.70                     | 0.56              |
| 8:AI:23:GLY:O     | 8:AI:24:ASN:HB2    | 2.04                     | 0.56              |
| 9:AJ:9:ARG:C      | 9:AJ:10:LEU:HD12   | 2.30                     | 0.56              |
| 9:AJ:52:LEU:HB2   | 13:AN:80:ARG:HD2   | 1.87                     | 0.56              |
| 16:AQ:56:ASP:HB3  | 16:AQ:79:GLU:O     | 2.05                     | 0.56              |
| 23:BB:1083:U:H1'  | 23:BB:1086:A:H61   | 1.70                     | 0.56              |
| 23:BB:1441:G:H2'  | 23:BB:1442:U:C6    | 2.40                     | 0.56              |
| 23:BB:1464:G:H2'  | 23:BB:1465:G:H8    | 1.68                     | 0.56              |
| 23:BB:1754:A:OP1  | 37:BP:95:LYS:HB2   | 2.04                     | 0.56              |
| 23:BB:1771:C:H2'  | 23:BB:1772:A:H8    | 1.69                     | 0.56              |
| 23:BB:2258:C:OP2  | 43:BW:3:LYS:HG3    | 2.05                     | 0.56              |
| 23:BB:2329:U:H2'  | 23:BB:2330:G:C8    | 2.40                     | 0.56              |
| 23:BB:2443:C:O2'  | 23:BB:2444:G:H5'   | 2.05                     | 0.56              |
| 24:BV:63:ILE:HD11 | 24:BV:72:VAL:HG21  | 1.87                     | 0.56              |
| 28:BF:108:PRO:HA  | 28:BF:113:PHE:CD1  | 2.40                     | 0.56              |
| 30:BH:2:GLN:N     | 30:BH:21:VAL:HG12  | 2.20                     | 0.56              |
| 31:BJ:10:THR:HG22 | 31:BJ:50:THR:N     | 2.20                     | 0.56              |
| 31:BJ:61:LYS:HE2  | 31:BJ:61:LYS:CA    | 2.35                     | 0.56              |
| 34:BM:41:LEU:HB2  | 34:BM:93:VAL:CG2   | 2.35                     | 0.56              |
| 34:BM:101:VAL:O   | 34:BM:102:LEU:HD12 | 2.05                     | 0.56              |
| 43:BW:43:LYS:HG2  | 43:BW:76:ARG:NH2   | 2.18                     | 0.56              |
| 46:BZ:25:ARG:HG3  | 46:BZ:26:SER:H     | 1.70                     | 0.56              |
| 49:B2:25:LYS:HE3  | 49:B2:25:LYS:H     | 1.68                     | 0.56              |
| 52:BI:85:ILE:CD1  | 52:BI:137:LEU:HD21 | 2.35                     | 0.56              |
| 52:BI:122:GLU:CD  | 52:BI:122:GLU:H    | 2.12                     | 0.56              |
| 1:CA:673:A:H1'    | 17:CR:63:TYR:CD1   | 2.39                     | 0.56              |
| 1:CA:784:A:H2'    | 1:CA:785:G:H8      | 1.70                     | 0.56              |
| 1:CA:940:C:H2'    | 1:CA:941:G:H8      | 1.70                     | 0.56              |
| 1:CA:1011:C:H2'   | 1:CA:1012:A:C8     | 2.40                     | 0.56              |
| 1:CA:1034:G:H2'   | 1:CA:1035:A:C8     | 2.40                     | 0.56              |
| 1:CA:1101:A:H61   | 20:CB:101:THR:HG21 | 1.70                     | 0.56              |
| 1:CA:1330:U:H2'   | 1:CA:1331:G:O4'    | 2.05                     | 0.56              |
| 2:CC:49:ALA:HB2   | 2:CC:74:ILE:CG2    | 2.34                     | 0.56              |
| 3:CD:84:ASN:ND2   | 3:CD:87:GLU:H      | 2.02                     | 0.56              |
| 9:CJ:53:ILE:HG13  | 13:CN:84:ARG:CZ    | 2.35                     | 0.56              |
| 14:CO:76:ARG:O    | 14:CO:79:ARG:HB2   | 2.05                     | 0.56              |
| 17:CR:23:LYS:HD2  | 17:CR:23:LYS:C     | 2.30                     | 0.56              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 17:CR:72:ARG:NH1   | 17:CR:72:ARG:HB2  | 2.19                     | 0.56              |
| 23:DB:175:G:H2'    | 23:DB:176:A:C8    | 2.40                     | 0.56              |
| 23:DB:241:A:O3'    | 23:DB:242:G:H4'   | 2.05                     | 0.56              |
| 23:DB:467:G:O2'    | 23:DB:468:G:H5'   | 2.05                     | 0.56              |
| 23:DB:479:A:OP1    | 23:DB:479:A:H4'   | 2.04                     | 0.56              |
| 23:DB:552:U:O2'    | 23:DB:553:G:H5'   | 2.05                     | 0.56              |
| 23:DB:1022:G:N2    | 23:DB:1142:A:N1   | 2.53                     | 0.56              |
| 23:DB:1560:G:H2'   | 23:DB:1561:C:H6   | 1.70                     | 0.56              |
| 23:DB:2025:C:OP1   | 26:DD:154:LYS:HE3 | 2.04                     | 0.56              |
| 23:DB:2061:G:H5''  | 23:DB:2503:A:C2   | 2.40                     | 0.56              |
| 26:DD:29:VAL:HG22  | 26:DD:30:GLU:N    | 2.13                     | 0.56              |
| 26:DD:69:ALA:HB1   | 26:DD:92:VAL:CG1  | 2.33                     | 0.56              |
| 27:DE:17:THR:HG23  | 27:DE:18:THR:H    | 1.67                     | 0.56              |
| 27:DE:149:ILE:HD13 | 27:DE:186:VAL:CG1 | 2.32                     | 0.56              |
| 28:DF:163:GLU:HG2  | 28:DF:166:ARG:CZ  | 2.35                     | 0.56              |
| 34:DM:6:ARG:HD2    | 34:DM:71:LYS:HE3  | 1.86                     | 0.56              |
| 35:DN:103:ARG:HG2  | 35:DN:106:ASP:OD2 | 2.05                     | 0.56              |
| 36:DO:108:ASP:O    | 36:DO:112:GLU:HG3 | 2.05                     | 0.56              |
| 41:DT:19:LYS:HZ3   | 41:DT:26:LYS:HE2  | 1.70                     | 0.56              |
| 43:DW:45:HIS:HB2   | 43:DW:66:VAL:HG11 | 1.87                     | 0.56              |
| 48:D1:19:PHE:CE2   | 48:D1:41:VAL:HG13 | 2.39                     | 0.56              |
| 1:AA:21:G:H2'      | 1:AA:22:G:C8      | 2.40                     | 0.56              |
| 1:AA:321:A:O2'     | 1:AA:322:C:H5'    | 2.05                     | 0.56              |
| 1:AA:1452:C:H5'    | 1:AA:1453:G:C4    | 2.40                     | 0.56              |
| 4:AE:45:VAL:O      | 4:AE:71:ILE:HG22  | 2.04                     | 0.56              |
| 4:AE:96:GLN:HB3    | 4:AE:123:LEU:CD1  | 2.36                     | 0.56              |
| 4:AE:104:ILE:HD11  | 4:AE:114:LEU:HB2  | 1.87                     | 0.56              |
| 4:AE:114:LEU:HD13  | 4:AE:122:VAL:HG21 | 1.88                     | 0.56              |
| 12:AM:53:ASP:OD1   | 12:AM:56:ARG:HD2  | 2.05                     | 0.56              |
| 19:AT:57:VAL:C     | 19:AT:60:GLN:HE22 | 2.13                     | 0.56              |
| 23:BB:1081:U:C5'   | 52:BI:126:ARG:HD2 | 2.35                     | 0.56              |
| 23:BB:1381:G:O2'   | 23:BB:1382:G:H5'  | 2.04                     | 0.56              |
| 23:BB:2297:A:N6    | 23:BB:2319:G:C3'  | 2.59                     | 0.56              |
| 23:BB:2590:A:H2'   | 23:BB:2591:C:C6   | 2.40                     | 0.56              |
| 23:BB:2621:G:HO2'  | 26:BD:164:GLN:HB2 | 1.69                     | 0.56              |
| 23:BB:2813:A:H2'   | 23:BB:2814:A:H8   | 1.70                     | 0.56              |
| 25:BC:164:VAL:HB   | 25:BC:167:ASP:CG  | 2.30                     | 0.56              |
| 27:BE:6:LYS:HG3    | 27:BE:9:GLN:HB2   | 1.86                     | 0.56              |
| 27:BE:74:LYS:O     | 27:BE:82:GLY:HA3  | 2.05                     | 0.56              |
| 32:BK:5:GLN:HA     | 32:BK:20:MET:SD   | 2.46                     | 0.56              |
| 35:BN:46:ARG:O     | 35:BN:50:PRO:HG2  | 2.06                     | 0.56              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 50:B3:4:LYS:NZ     | 50:B3:59:ALA:H    | 2.03                     | 0.56              |
| 1:CA:1329:A:O2'    | 1:CA:1330:U:H5'   | 2.05                     | 0.56              |
| 2:CC:39:ARG:NH2    | 13:CN:91:GLU:HB3  | 2.19                     | 0.56              |
| 5:CF:2:ARG:HH11    | 5:CF:2:ARG:HB3    | 1.71                     | 0.56              |
| 6:CG:29:LEU:HD23   | 6:CG:104:VAL:HG13 | 1.87                     | 0.56              |
| 9:CJ:9:ARG:HB2     | 9:CJ:99:GLN:H     | 1.70                     | 0.56              |
| 9:CJ:30:LYS:O      | 9:CJ:30:LYS:HD3   | 2.04                     | 0.56              |
| 12:CM:15:VAL:O     | 12:CM:19:THR:HG23 | 2.05                     | 0.56              |
| 13:CN:29:ILE:HG22  | 13:CN:30:ILE:N    | 2.20                     | 0.56              |
| 22:DA:75:G:H5''    | 24:DV:12:GLN:OE1  | 2.05                     | 0.56              |
| 23:DB:69:C:H2'     | 23:DB:70:G:C8     | 2.40                     | 0.56              |
| 23:DB:609:A:H2'    | 23:DB:610:C:O4'   | 2.05                     | 0.56              |
| 23:DB:660:C:H2'    | 23:DB:661:A:C8    | 2.39                     | 0.56              |
| 23:DB:1061:U:O4'   | 23:DB:1070:A:H1'  | 2.04                     | 0.56              |
| 23:DB:2150:C:H2'   | 23:DB:2151:U:C6   | 2.39                     | 0.56              |
| 23:DB:2250:G:N2    | 23:DB:2496:C:H4'  | 2.20                     | 0.56              |
| 23:DB:2285:C:H5    | 48:D1:7:LYS:HE3   | 1.70                     | 0.56              |
| 23:DB:2813:A:H2'   | 23:DB:2814:A:H8   | 1.70                     | 0.56              |
| 25:DC:208:GLY:HA2  | 25:DC:212:TRP:CB  | 2.35                     | 0.56              |
| 26:DD:156:PHE:CD1  | 31:DJ:81:ILE:HG21 | 2.41                     | 0.56              |
| 27:DE:126:VAL:HG21 | 27:DE:132:LYS:NZ  | 2.19                     | 0.56              |
| 28:DF:4:HIS:O      | 28:DF:7:TYR:HB3   | 2.05                     | 0.56              |
| 29:DG:6:ALA:HB3    | 29:DG:7:PRO:HD3   | 1.87                     | 0.56              |
| 39:DR:76:LYS:HA    | 39:DR:91:GLN:H    | 1.70                     | 0.56              |
| 41:DT:76:ARG:HG2   | 41:DT:77:ARG:N    | 2.20                     | 0.56              |
| 1:AA:218:U:H2'     | 1:AA:219:U:C6     | 2.40                     | 0.56              |
| 1:AA:384:G:H2'     | 1:AA:385:C:H6     | 1.69                     | 0.56              |
| 1:AA:429:U:H1'     | 1:AA:430:A:H5''   | 1.87                     | 0.56              |
| 1:AA:477:C:H2'     | 1:AA:478:A:C8     | 2.41                     | 0.56              |
| 1:AA:674:G:H2'     | 1:AA:675:A:C8     | 2.40                     | 0.56              |
| 1:AA:677:U:H2'     | 1:AA:678:U:H6     | 1.70                     | 0.56              |
| 1:AA:930:C:H2'     | 1:AA:931:C:O4'    | 2.05                     | 0.56              |
| 1:AA:1040:U:H2'    | 1:AA:1041:G:C8    | 2.40                     | 0.56              |
| 2:AC:33:ASP:HB2    | 13:AN:64:ARG:HD3  | 1.86                     | 0.56              |
| 2:AC:146:LYS:HE3   | 2:AC:202:PHE:CE2  | 2.38                     | 0.56              |
| 5:AF:55:HIS:O      | 5:AF:56:LYS:HG3   | 2.06                     | 0.56              |
| 5:AF:100:SER:HA    | 17:AR:23:LYS:NZ   | 2.19                     | 0.56              |
| 9:AJ:53:ILE:HG23   | 13:AN:84:ARG:CZ   | 2.36                     | 0.56              |
| 9:AJ:55:PRO:O      | 9:AJ:56:HIS:HB3   | 2.06                     | 0.56              |
| 10:AK:25:SER:HB3   | 10:AK:28:ASN:O    | 2.06                     | 0.56              |
| 12:AM:13:HIS:HB2   | 12:AM:16:ILE:CG2  | 2.36                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:AN:60:ARG:NH2   | 13:AN:62:ARG:HE    | 2.02                     | 0.56              |
| 17:AR:41:SER:HB2   | 17:AR:51:GLN:HG2   | 1.87                     | 0.56              |
| 21:AU:13:VAL:HG13  | 21:AU:14:ALA:N     | 2.12                     | 0.56              |
| 23:BB:125:A:H4'    | 49:B2:13:ASN:OD1   | 2.05                     | 0.56              |
| 23:BB:328:U:H4'    | 42:BU:65:GLN:CG    | 2.35                     | 0.56              |
| 23:BB:796:C:H2'    | 23:BB:797:G:C8     | 2.40                     | 0.56              |
| 23:BB:1082:U:C2    | 23:BB:1086:A:C6    | 2.93                     | 0.56              |
| 23:BB:1250:G:H5''  | 38:BQ:5:ARG:HG2    | 1.86                     | 0.56              |
| 23:BB:1528:A:H2'   | 23:BB:1529:G:O4'   | 2.06                     | 0.56              |
| 23:BB:1695:G:H1'   | 25:BC:14:HIS:O     | 2.05                     | 0.56              |
| 23:BB:1709:U:H2'   | 23:BB:1710:G:C8    | 2.41                     | 0.56              |
| 23:BB:1729:U:H2'   | 23:BB:1730:C:H4'   | 1.87                     | 0.56              |
| 23:BB:2869:G:H2'   | 23:BB:2870:C:C6    | 2.40                     | 0.56              |
| 24:BV:9:ARG:HH12   | 24:BV:27:PRO:HA    | 1.69                     | 0.56              |
| 24:BV:76:ASP:HB2   | 34:BM:136:MET:HE3  | 1.87                     | 0.56              |
| 25:BC:68:ARG:NH2   | 25:BC:190:THR:HG23 | 2.20                     | 0.56              |
| 25:BC:174:ARG:HG3  | 25:BC:180:MET:SD   | 2.44                     | 0.56              |
| 26:BD:5:VAL:HB     | 26:BD:27:ILE:O     | 2.05                     | 0.56              |
| 26:BD:201:LEU:HD12 | 26:BD:201:LEU:N    | 2.19                     | 0.56              |
| 27:BE:28:VAL:O     | 27:BE:32:VAL:HG23  | 2.06                     | 0.56              |
| 27:BE:120:VAL:N    | 27:BE:189:THR:HG22 | 2.20                     | 0.56              |
| 27:BE:148:ILE:H    | 27:BE:183:PHE:HB3  | 1.70                     | 0.56              |
| 28:BF:116:LEU:HD12 | 28:BF:176:PHE:CD2  | 2.40                     | 0.56              |
| 28:BF:170:ALA:HA   | 28:BF:173:ASP:OD1  | 2.04                     | 0.56              |
| 29:BG:132:LEU:HD11 | 29:BG:144:ALA:HB2  | 1.88                     | 0.56              |
| 31:BJ:18:VAL:CG2   | 31:BJ:56:VAL:HA    | 2.35                     | 0.56              |
| 34:BM:3:GLN:N      | 34:BM:4:PRO:CD     | 2.63                     | 0.56              |
| 38:BQ:65:ASN:O     | 38:BQ:69:ARG:HG2   | 2.06                     | 0.56              |
| 39:BR:43:ASN:C     | 39:BR:45:GLU:H     | 2.11                     | 0.56              |
| 41:BT:68:LYS:NZ    | 41:BT:73:ARG:HA    | 2.20                     | 0.56              |
| 48:B1:9:LYS:HG2    | 50:B3:34:LYS:HZ3   | 1.70                     | 0.56              |
| 50:B3:44:ARG:CG    | 50:B3:45:PRO:HD2   | 2.34                     | 0.56              |
| 1:CA:266:G:O2'     | 1:CA:267:C:H3'     | 2.06                     | 0.56              |
| 1:CA:477:C:H2'     | 1:CA:478:A:C8      | 2.41                     | 0.56              |
| 1:CA:586:C:C2'     | 1:CA:587:G:H5'     | 2.36                     | 0.56              |
| 1:CA:981:U:H2'     | 1:CA:982:U:C5      | 2.40                     | 0.56              |
| 3:CD:162:GLU:HG3   | 3:CD:163:GLN:HE21  | 1.70                     | 0.56              |
| 3:CD:192:ALA:HB3   | 3:CD:194:ILE:HG22  | 1.87                     | 0.56              |
| 6:CG:55:LYS:HG3    | 6:CG:56:SER:H      | 1.70                     | 0.56              |
| 8:CI:78:ILE:O      | 8:CI:82:ILE:HG13   | 2.04                     | 0.56              |
| 11:CL:23:LEU:C     | 11:CL:25:ALA:H     | 2.13                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:CM:106:ARG:N   | 12:CM:106:ARG:HH11 | 2.04                     | 0.56              |
| 19:CT:57:VAL:HG12 | 19:CT:71:ALA:HB1   | 1.86                     | 0.56              |
| 23:DB:3:U:H2'     | 23:DB:4:U:H6       | 1.70                     | 0.56              |
| 23:DB:17:G:H2'    | 23:DB:18:U:C6      | 2.40                     | 0.56              |
| 23:DB:91:A:H1'    | 23:DB:92:U:C6      | 2.41                     | 0.56              |
| 23:DB:131:A:H2'   | 23:DB:132:G:H8     | 1.70                     | 0.56              |
| 23:DB:155:A:H2'   | 23:DB:156:A:C8     | 2.41                     | 0.56              |
| 23:DB:171:U:H2'   | 23:DB:172:A:C8     | 2.40                     | 0.56              |
| 23:DB:172:A:H2'   | 23:DB:173:A:H8     | 1.70                     | 0.56              |
| 23:DB:234:U:O2'   | 23:DB:235:U:H5'    | 2.04                     | 0.56              |
| 23:DB:351:C:H2'   | 23:DB:352:A:H8     | 1.69                     | 0.56              |
| 23:DB:490:C:H3'   | 23:DB:491:G:H5''   | 1.87                     | 0.56              |
| 23:DB:527:C:O4'   | 23:DB:527:C:O2     | 2.21                     | 0.56              |
| 23:DB:877:A:N6    | 23:DB:898:C:H2'    | 2.19                     | 0.56              |
| 23:DB:975:A:H5'   | 39:DR:83:TYR:OH    | 2.05                     | 0.56              |
| 23:DB:1327:A:H2'  | 23:DB:1328:A:O4'   | 2.06                     | 0.56              |
| 23:DB:1381:G:H2'  | 23:DB:1382:G:H5'   | 1.86                     | 0.56              |
| 23:DB:1661:G:O2'  | 23:DB:1662:U:H5'   | 2.05                     | 0.56              |
| 23:DB:1709:U:H2'  | 23:DB:1710:G:C8    | 2.40                     | 0.56              |
| 23:DB:1771:C:H2'  | 23:DB:1772:A:H8    | 1.69                     | 0.56              |
| 23:DB:1826:G:H2'  | 23:DB:1827:U:H6    | 1.69                     | 0.56              |
| 23:DB:1917:U:O2'  | 23:DB:1918:A:H5'   | 2.06                     | 0.56              |
| 23:DB:2140:G:H2'  | 23:DB:2141:G:O4'   | 2.04                     | 0.56              |
| 23:DB:2233:U:H2'  | 23:DB:2234:G:H8    | 1.69                     | 0.56              |
| 23:DB:2626:C:O2'  | 23:DB:2627:G:H5'   | 2.05                     | 0.56              |
| 23:DB:2872:A:O2'  | 23:DB:2873:A:H5''  | 2.05                     | 0.56              |
| 23:DB:2882:A:H2'  | 23:DB:2883:A:H5''  | 1.86                     | 0.56              |
| 23:DB:2898:U:H2'  | 23:DB:2899:A:H8    | 1.70                     | 0.56              |
| 25:DC:79:ARG:HD2  | 25:DC:110:LYS:HE2  | 1.87                     | 0.56              |
| 26:DD:8:LYS:CE    | 37:DP:5:LYS:HG3    | 2.34                     | 0.56              |
| 26:DD:201:LEU:O   | 26:DD:202:ILE:HD12 | 2.05                     | 0.56              |
| 27:DE:6:LYS:CD    | 27:DE:7:ASP:H      | 2.16                     | 0.56              |
| 27:DE:190:ALA:HB3 | 27:DE:193:VAL:HG22 | 1.86                     | 0.56              |
| 28:DF:3:LEU:O     | 28:DF:3:LEU:HD23   | 2.05                     | 0.56              |
| 28:DF:79:ARG:HB2  | 28:DF:82:TYR:CE2   | 2.40                     | 0.56              |
| 28:DF:163:GLU:HA  | 28:DF:166:ARG:HD2  | 1.87                     | 0.56              |
| 31:DJ:25:LEU:HD13 | 31:DJ:25:LEU:N     | 2.20                     | 0.56              |
| 32:DK:113:MET:CE  | 32:DK:116:ILE:HD11 | 2.35                     | 0.56              |
| 33:DL:92:LEU:HD13 | 33:DL:96:LYS:HG2   | 1.87                     | 0.56              |
| 35:DN:4:ARG:HG2   | 35:DN:5:LYS:N      | 2.19                     | 0.56              |
| 35:DN:86:ARG:NH2  | 35:DN:117:ASP:HA   | 2.20                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:DP:90:ALA:N     | 37:DP:112:ARG:HH21 | 2.01                     | 0.56              |
| 39:DR:11:GLN:C     | 39:DR:21:ARG:HH22  | 2.14                     | 0.56              |
| 39:DR:67:GLY:H     | 39:DR:98:ILE:HA    | 1.69                     | 0.56              |
| 40:DS:28:LYS:HA    | 40:DS:31:GLN:NE2   | 2.19                     | 0.56              |
| 40:DS:46:LEU:O     | 40:DS:50:VAL:HG13  | 2.06                     | 0.56              |
| 40:DS:85:ILE:HD13  | 40:DS:85:ILE:C     | 2.31                     | 0.56              |
| 45:DY:43:ILE:HA    | 45:DY:46:MET:HE2   | 1.86                     | 0.56              |
| 1:AA:77:A:H2'      | 1:AA:78:A:C8       | 2.40                     | 0.56              |
| 1:AA:301:G:H2'     | 1:AA:302:G:H8      | 1.71                     | 0.56              |
| 1:AA:499:A:H4'     | 1:AA:500:G:OP1     | 2.06                     | 0.56              |
| 19:AT:82:ILE:HG13  | 19:AT:83:ASN:N     | 2.20                     | 0.56              |
| 20:AB:76:SER:HA    | 20:AB:92:ASN:HB2   | 1.87                     | 0.56              |
| 20:AB:195:VAL:HG12 | 20:AB:197:PHE:H    | 1.70                     | 0.56              |
| 22:BA:26:C:H2'     | 22:BA:27:C:O4'     | 2.06                     | 0.56              |
| 23:BB:189:G:OP1    | 46:BZ:24:ILE:HD12  | 2.05                     | 0.56              |
| 23:BB:458:G:H5''   | 49:B2:39:ARG:O     | 2.04                     | 0.56              |
| 23:BB:962:G:H21    | 23:BB:2250:G:H1    | 1.53                     | 0.56              |
| 23:BB:1061:U:O4'   | 23:BB:1070:A:H1'   | 2.05                     | 0.56              |
| 23:BB:1351:C:O2'   | 23:BB:1571:A:H1'   | 2.06                     | 0.56              |
| 23:BB:1459:G:C2'   | 23:BB:1460:U:H5'   | 2.35                     | 0.56              |
| 23:BB:1938:A:O2'   | 23:BB:1939:U:H5''  | 2.06                     | 0.56              |
| 23:BB:2022:U:O2'   | 23:BB:2617:U:H5'   | 2.06                     | 0.56              |
| 23:BB:2053:G:H5''  | 26:BD:150:GLN:HA   | 1.86                     | 0.56              |
| 23:BB:2147:A:H5'   | 23:BB:2148:G:H4'   | 1.87                     | 0.56              |
| 28:BF:83:PRO:HG2   | 28:BF:84:ILE:H     | 1.71                     | 0.56              |
| 30:BH:80:ILE:HD12  | 30:BH:102:ALA:HB2  | 1.88                     | 0.56              |
| 31:BJ:16:TYR:O     | 31:BJ:55:ILE:HG22  | 2.04                     | 0.56              |
| 31:BJ:58:ASN:HA    | 31:BJ:127:GLY:N    | 2.21                     | 0.56              |
| 33:BL:80:SER:O     | 33:BL:116:VAL:HA   | 2.06                     | 0.56              |
| 33:BL:119:PRO:O    | 33:BL:119:PRO:HD2  | 2.05                     | 0.56              |
| 34:BM:33:LEU:HB2   | 34:BM:101:VAL:CG2  | 2.35                     | 0.56              |
| 38:BQ:34:ALA:O     | 38:BQ:38:VAL:HG12  | 2.06                     | 0.56              |
| 38:BQ:79:ILE:HA    | 38:BQ:82:LEU:HD12  | 1.87                     | 0.56              |
| 39:BR:66:HIS:H     | 39:BR:98:ILE:HD13  | 1.70                     | 0.56              |
| 48:B1:53:ILE:HD13  | 48:B1:54:LYS:H     | 1.70                     | 0.56              |
| 50:B3:41:ARG:NH1   | 50:B3:42:HIS:HB3   | 2.20                     | 0.56              |
| 1:CA:474:G:H2'     | 1:CA:475:C:C6      | 2.40                     | 0.56              |
| 1:CA:815:A:H62     | 1:CA:1509:C:H1'    | 1.70                     | 0.56              |
| 1:CA:1314:C:OP2    | 18:CS:5:LYS:HG2    | 2.05                     | 0.56              |
| 1:CA:1470:U:O2'    | 1:CA:1471:U:H5'    | 2.05                     | 0.56              |
| 10:CK:22:ILE:HD13  | 10:CK:95:THR:HG23  | 1.87                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 15:CP:52:LEU:HD21 | 15:CP:74:LEU:HB2   | 1.87                     | 0.56              |
| 20:CB:78:ALA:HB1  | 20:CB:213:LEU:HD13 | 1.87                     | 0.56              |
| 23:DB:144:A:H8    | 23:DB:144:A:O5'    | 1.89                     | 0.56              |
| 23:DB:323:C:C1'   | 27:DE:164:LEU:HB3  | 2.25                     | 0.56              |
| 23:DB:876:C:H3'   | 23:DB:877:A:O4'    | 2.06                     | 0.56              |
| 23:DB:2090:A:O2'  | 46:DZ:49:ARG:CD    | 2.53                     | 0.56              |
| 23:DB:2262:U:OP2  | 43:DW:13:ARG:HD3   | 2.04                     | 0.56              |
| 25:DC:128:THR:HA  | 25:DC:190:THR:HA   | 1.86                     | 0.56              |
| 25:DC:179:GLU:HB3 | 25:DC:266:ILE:HA   | 1.88                     | 0.56              |
| 28:DF:174:PHE:H   | 28:DF:175:PRO:CD   | 2.19                     | 0.56              |
| 42:DU:25:LYS:O    | 42:DU:34:ILE:HG12  | 2.06                     | 0.56              |
| 43:DW:38:ARG:HG3  | 43:DW:39:GLN:N     | 2.21                     | 0.56              |
| 46:DZ:49:ARG:C    | 46:DZ:51:VAL:N     | 2.61                     | 0.56              |
| 50:D3:4:LYS:HE3   | 50:D3:61:LEU:HD13  | 1.88                     | 0.56              |
| 52:DI:24:GLY:HA2  | 52:DI:34:ILE:HD12  | 1.86                     | 0.56              |
| 1:AA:474:G:H2'    | 1:AA:475:C:C6      | 2.40                     | 0.56              |
| 1:AA:586:C:C2'    | 1:AA:587:G:H5'     | 2.35                     | 0.56              |
| 1:AA:1225:A:H3'   | 1:AA:1226:C:C6     | 2.40                     | 0.56              |
| 1:AA:1329:A:O2'   | 1:AA:1330:U:H5'    | 2.05                     | 0.56              |
| 1:AA:1463:U:H2'   | 1:AA:1464:U:C6     | 2.40                     | 0.56              |
| 1:AA:1470:U:O2'   | 1:AA:1471:U:H5'    | 2.06                     | 0.56              |
| 3:AD:117:VAL:O    | 3:AD:130:ASN:HA    | 2.05                     | 0.56              |
| 6:AG:22:LEU:O     | 6:AG:25:PHE:HB3    | 2.06                     | 0.56              |
| 6:AG:91:ARG:HB3   | 6:AG:92:PRO:HD2    | 1.88                     | 0.56              |
| 14:AO:63:ARG:HA   | 14:AO:66:LEU:HD12  | 1.87                     | 0.56              |
| 18:AS:48:ILE:HD12 | 18:AS:48:ILE:N     | 2.21                     | 0.56              |
| 19:AT:61:ALA:HA   | 19:AT:66:ILE:O     | 2.05                     | 0.56              |
| 20:AB:163:ILE:CG2 | 20:AB:164:ASP:H    | 1.96                     | 0.56              |
| 23:BB:2:G:O2'     | 23:BB:3:U:H5'      | 2.05                     | 0.56              |
| 23:BB:535:G:O2'   | 38:BQ:52:ARG:HD3   | 2.05                     | 0.56              |
| 23:BB:597:G:H4'   | 33:BL:21:ARG:NE    | 2.18                     | 0.56              |
| 23:BB:851:C:O2'   | 45:BY:45:GLY:HA3   | 2.05                     | 0.56              |
| 23:BB:1661:G:O2'  | 23:BB:1662:U:H5'   | 2.05                     | 0.56              |
| 23:BB:1826:G:H2'  | 23:BB:1827:U:H6    | 1.70                     | 0.56              |
| 23:BB:1842:G:H2'  | 23:BB:1843:C:H6    | 1.70                     | 0.56              |
| 23:BB:1889:A:H2'  | 23:BB:1890:A:C8    | 2.41                     | 0.56              |
| 23:BB:2729:G:H2'  | 23:BB:2730:C:C6    | 2.41                     | 0.56              |
| 23:BB:2747:G:O6   | 23:BB:2755:C:H5''  | 2.05                     | 0.56              |
| 23:BB:2840:C:H5'' | 35:BN:53:THR:CG2   | 2.36                     | 0.56              |
| 33:BL:118:THR:N   | 33:BL:119:PRO:CD   | 2.66                     | 0.56              |
| 34:BM:41:LEU:HG   | 34:BM:95:LEU:HD12  | 1.86                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:BM:96:ILE:HD13 | 34:BM:97:GLN:N    | 2.21                     | 0.56              |
| 36:BO:8:ILE:HG23  | 36:BO:9:ARG:N     | 2.20                     | 0.56              |
| 37:BP:47:ILE:HG23 | 37:BP:63:ILE:HG13 | 1.88                     | 0.56              |
| 38:BQ:22:GLY:O    | 38:BQ:24:TYR:N    | 2.39                     | 0.56              |
| 38:BQ:50:ARG:O    | 38:BQ:53:LYS:HD3  | 2.05                     | 0.56              |
| 41:BT:96:VAL:HG22 | 41:BT:97:GLY:N    | 2.21                     | 0.56              |
| 52:BI:10:LEU:O    | 52:BI:10:LEU:HD12 | 2.05                     | 0.56              |
| 1:CA:218:U:H2'    | 1:CA:219:U:C6     | 2.40                     | 0.56              |
| 1:CA:429:U:H1'    | 1:CA:430:A:H5''   | 1.87                     | 0.56              |
| 1:CA:764:C:H2'    | 1:CA:765:G:H5'    | 1.88                     | 0.56              |
| 1:CA:1228:C:H5'   | 12:CM:112:ARG:HB3 | 1.87                     | 0.56              |
| 1:CA:1313:U:P     | 18:CS:5:LYS:HA    | 2.46                     | 0.56              |
| 6:CG:2:ARG:HH11   | 6:CG:2:ARG:CB     | 2.17                     | 0.56              |
| 9:CJ:9:ARG:HB3    | 9:CJ:99:GLN:HE21  | 1.70                     | 0.56              |
| 23:DB:287:G:H2'   | 23:DB:288:U:C6    | 2.40                     | 0.56              |
| 23:DB:818:G:H5'   | 23:DB:839:U:OP1   | 2.06                     | 0.56              |
| 23:DB:1316:U:O2'  | 23:DB:1317:G:H5'  | 2.05                     | 0.56              |
| 23:DB:2360:G:O2'  | 33:DL:61:LEU:HD21 | 2.06                     | 0.56              |
| 23:DB:2527:C:H1'  | 51:D4:1:MET:HG3   | 1.87                     | 0.56              |
| 23:DB:2600:A:O2'  | 23:DB:2601:C:H5'  | 2.05                     | 0.56              |
| 23:DB:2729:G:H2'  | 23:DB:2730:C:C6   | 2.41                     | 0.56              |
| 23:DB:2758:A:O2'  | 23:DB:2759:G:H5'  | 2.04                     | 0.56              |
| 23:DB:2798:U:H1'  | 23:DB:2800:A:N6   | 2.20                     | 0.56              |
| 25:DC:156:SER:O   | 25:DC:158:GLY:N   | 2.39                     | 0.56              |
| 26:DD:159:LYS:O   | 26:DD:160:LYS:HB2 | 2.05                     | 0.56              |
| 27:DE:184:ASP:CB  | 33:DL:13:LYS:HE3  | 2.36                     | 0.56              |
| 31:DJ:7:LYS:HD2   | 31:DJ:45:THR:CB   | 2.35                     | 0.56              |
| 36:DO:15:ARG:NH1  | 43:DW:76:ARG:HE   | 2.03                     | 0.56              |
| 37:DP:28:LYS:HD3  | 37:DP:44:GLY:CA   | 2.33                     | 0.56              |
| 41:DT:34:VAL:HG21 | 41:DT:43:ILE:CD1  | 2.33                     | 0.56              |
| 42:DU:21:ARG:HH11 | 42:DU:21:ARG:HG3  | 1.70                     | 0.56              |
| 46:DZ:41:HIS:ND1  | 46:DZ:42:PRO:HD2  | 2.20                     | 0.56              |
| 1:AA:327:A:H1'    | 1:AA:329:A:O4'    | 2.06                     | 0.56              |
| 1:AA:956:U:O2'    | 1:AA:957:U:H5'    | 2.06                     | 0.56              |
| 1:AA:1310:G:H2'   | 1:AA:1311:A:O4'   | 2.06                     | 0.56              |
| 1:AA:1432:G:H5''  | 37:BP:106:ALA:HB2 | 1.88                     | 0.56              |
| 1:AA:1468:A:O2'   | 1:AA:1469:C:H5'   | 2.05                     | 0.56              |
| 3:AD:10:LEU:HD21  | 3:AD:62:ARG:CD    | 2.36                     | 0.56              |
| 8:AI:38:PHE:O     | 8:AI:41:GLU:HB2   | 2.06                     | 0.56              |
| 10:AK:92:ARG:HH11 | 10:AK:92:ARG:CB   | 2.19                     | 0.56              |
| 20:AB:53:LEU:HD21 | 20:AB:212:TYR:HE2 | 1.70                     | 0.56              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 20:AB:144:GLU:O   | 20:AB:148:GLY:HA3  | 2.05                     | 0.56              |
| 22:BA:90:C:H2'    | 22:BA:91:C:O4'     | 2.05                     | 0.56              |
| 23:BB:988:A:H4'   | 23:BB:1155:A:N1    | 2.21                     | 0.56              |
| 23:BB:1133:A:H4'  | 23:BB:1134:A:H5''  | 1.87                     | 0.56              |
| 23:BB:1750:G:O2'  | 23:BB:1751:U:H5'   | 2.06                     | 0.56              |
| 23:BB:1754:A:P    | 37:BP:94:ALA:HB1   | 2.46                     | 0.56              |
| 23:BB:2052:A:H5'  | 26:BD:148:GLN:O    | 2.05                     | 0.56              |
| 23:BB:2239:G:H5'  | 25:BC:246:PRO:HD2  | 1.87                     | 0.56              |
| 23:BB:2586:U:H2'  | 23:BB:2587:A:C8    | 2.41                     | 0.56              |
| 23:BB:2665:A:O2'  | 23:BB:2666:C:H5'   | 2.06                     | 0.56              |
| 23:BB:2798:U:H1'  | 23:BB:2800:A:N6    | 2.20                     | 0.56              |
| 27:BE:128:ALA:O   | 27:BE:157:LEU:HB2  | 2.05                     | 0.56              |
| 31:BJ:102:GLU:HG3 | 31:BJ:124:VAL:HG11 | 1.87                     | 0.56              |
| 39:BR:66:HIS:HA   | 39:BR:98:ILE:HD13  | 1.86                     | 0.56              |
| 39:BR:90:ARG:HH22 | 39:BR:92:TRP:HB3   | 1.69                     | 0.56              |
| 40:BS:8:ARG:CZ    | 40:BS:102:HIS:NE2  | 2.69                     | 0.56              |
| 40:BS:9:HIS:O     | 40:BS:100:THR:HB   | 2.04                     | 0.56              |
| 40:BS:47:VAL:O    | 40:BS:51:LEU:HB2   | 2.05                     | 0.56              |
| 41:BT:30:ILE:HG22 | 41:BT:84:TYR:O     | 2.06                     | 0.56              |
| 41:BT:40:LYS:HB3  | 41:BT:58:VAL:HB    | 1.88                     | 0.56              |
| 45:BY:13:ILE:HG23 | 45:BY:19:HIS:HE1   | 1.70                     | 0.56              |
| 1:CA:642:A:C5     | 7:CH:106:SER:HA    | 2.41                     | 0.56              |
| 1:CA:1250:A:H5''  | 8:CI:69:GLY:N      | 2.21                     | 0.56              |
| 1:CA:1262:C:H2'   | 1:CA:1263:C:H6     | 1.70                     | 0.56              |
| 3:CD:106:PHE:CD1  | 3:CD:158:LEU:HD21  | 2.41                     | 0.56              |
| 10:CK:78:ILE:H    | 10:CK:78:ILE:CD1   | 2.06                     | 0.56              |
| 23:DB:171:U:H2'   | 23:DB:172:A:H8     | 1.71                     | 0.56              |
| 23:DB:388:G:N7    | 23:DB:390:U:H2'    | 2.20                     | 0.56              |
| 23:DB:659:G:H21   | 27:DE:30:GLN:NE2   | 2.03                     | 0.56              |
| 23:DB:1018:U:O2'  | 23:DB:1019:U:H5'   | 2.05                     | 0.56              |
| 23:DB:1528:A:H2'  | 23:DB:1529:G:O4'   | 2.06                     | 0.56              |
| 23:DB:1750:G:O2'  | 23:DB:1751:U:H5'   | 2.06                     | 0.56              |
| 23:DB:1796:U:OP1  | 25:DC:269:ARG:HD3  | 2.06                     | 0.56              |
| 24:DV:9:ARG:NH2   | 24:DV:20:LEU:HD11  | 2.20                     | 0.56              |
| 27:DE:17:THR:HG23 | 27:DE:18:THR:N     | 2.21                     | 0.56              |
| 27:DE:85:PHE:O    | 27:DE:86:ALA:HB2   | 2.06                     | 0.56              |
| 27:DE:195:GLN:HB2 | 27:DE:198:GLU:O    | 2.06                     | 0.56              |
| 30:DH:58:LEU:O    | 30:DH:61:VAL:HG22  | 2.05                     | 0.56              |
| 30:DH:82:SER:O    | 30:DH:83:LYS:HD2   | 2.05                     | 0.56              |
| 33:DL:78:ARG:CZ   | 33:DL:113:ALA:HB1  | 2.36                     | 0.56              |
| 33:DL:132:ARG:NH1 | 33:DL:140:GLY:HA2  | 2.21                     | 0.56              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:DY:4:ILE:HG12   | 45:DY:5:LYS:HG3    | 1.87                     | 0.56              |
| 50:D3:24:LYS:HB3   | 50:D3:24:LYS:HZ2   | 1.71                     | 0.56              |
| 1:AA:449:G:H2'     | 1:AA:450:G:C8      | 2.40                     | 0.56              |
| 1:AA:552:U:H2'     | 1:AA:553:A:C8      | 2.41                     | 0.56              |
| 2:AC:133:MET:HE2   | 2:AC:152:VAL:CG2   | 2.34                     | 0.56              |
| 4:AE:87:VAL:HG11   | 4:AE:92:ARG:HD3    | 1.87                     | 0.56              |
| 6:AG:14:ASP:CG     | 6:AG:15:PRO:HD2    | 2.31                     | 0.56              |
| 11:AL:106:VAL:HG21 | 11:AL:109:ARG:HG3  | 1.88                     | 0.56              |
| 18:AS:62:THR:N     | 18:AS:65:MET:HE3   | 2.21                     | 0.56              |
| 23:BB:1971:U:H1'   | 25:BC:238:ASN:ND2  | 2.20                     | 0.56              |
| 23:BB:2065:C:H2'   | 23:BB:2066:C:H6    | 1.71                     | 0.56              |
| 23:BB:2262:U:H2'   | 23:BB:2263:C:H6    | 1.71                     | 0.56              |
| 23:BB:2484:G:H1'   | 34:BM:119:LEU:HD12 | 1.87                     | 0.56              |
| 24:BV:44:HIS:HE2   | 24:BV:85:LYS:HB2   | 1.71                     | 0.56              |
| 26:BD:8:LYS:HA     | 26:BD:197:THR:HG23 | 1.88                     | 0.56              |
| 28:BF:7:TYR:O      | 28:BF:11:VAL:HB    | 2.05                     | 0.56              |
| 28:BF:66:ILE:HA    | 28:BF:85:GLY:O     | 2.06                     | 0.56              |
| 29:BG:84:LYS:HZ3   | 29:BG:84:LYS:HA    | 1.70                     | 0.56              |
| 30:BH:69:ALA:HB2   | 30:BH:140:ALA:HA   | 1.86                     | 0.56              |
| 31:BJ:57:LEU:HD12  | 31:BJ:128:ASN:C    | 2.31                     | 0.56              |
| 33:BL:106:GLU:CD   | 33:BL:106:GLU:H    | 2.12                     | 0.56              |
| 35:BN:32:GLU:HB3   | 35:BN:33:ILE:HD13  | 1.88                     | 0.56              |
| 35:BN:73:ASN:N     | 35:BN:73:ASN:HD22  | 2.03                     | 0.56              |
| 39:BR:42:ALA:HB1   | 39:BR:45:GLU:OE2   | 2.05                     | 0.56              |
| 41:BT:30:ILE:HG23  | 41:BT:32:LEU:HD13  | 1.87                     | 0.56              |
| 41:BT:50:LEU:C     | 41:BT:52:GLU:H     | 2.13                     | 0.56              |
| 43:BW:39:GLN:HG2   | 43:BW:68:PHE:HB2   | 1.86                     | 0.56              |
| 1:CA:321:A:O2'     | 1:CA:322:C:H5'     | 2.06                     | 0.56              |
| 1:CA:327:A:H1'     | 1:CA:329:A:O4'     | 2.06                     | 0.56              |
| 1:CA:591:U:H2'     | 1:CA:592:G:H8      | 1.70                     | 0.56              |
| 5:CF:47:LEU:HD22   | 17:CR:65:SER:OG    | 2.05                     | 0.56              |
| 6:CG:24:LYS:O      | 6:CG:28:ILE:HG12   | 2.06                     | 0.56              |
| 11:CL:107:LYS:O    | 11:CL:108:ASP:HB2  | 2.06                     | 0.56              |
| 13:CN:41:TRP:O     | 13:CN:45:LEU:HG    | 2.06                     | 0.56              |
| 23:DB:4:U:O2'      | 23:DB:5:A:H5'      | 2.05                     | 0.56              |
| 23:DB:374:A:H61    | 23:DB:400:G:H1'    | 1.68                     | 0.56              |
| 23:DB:1862:G:O2'   | 23:DB:1863:G:H5'   | 2.06                     | 0.56              |
| 23:DB:1878:G:H2'   | 23:DB:1879:C:H6    | 1.69                     | 0.56              |
| 23:DB:2405:G:H5''  | 33:DL:70:LYS:HG3   | 1.86                     | 0.56              |
| 23:DB:2639:A:H2'   | 23:DB:2640:G:O4'   | 2.06                     | 0.56              |
| 23:DB:2839:G:H2'   | 23:DB:2840:C:H6    | 1.69                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DC:224:MET:HA   | 25:DC:233:GLY:N    | 2.13                     | 0.56              |
| 25:DC:254:LYS:N    | 25:DC:254:LYS:HD2  | 2.21                     | 0.56              |
| 26:DD:25:THR:HG22  | 26:DD:188:LEU:HG   | 1.88                     | 0.56              |
| 26:DD:35:THR:HB    | 26:DD:48:ILE:HG13  | 1.87                     | 0.56              |
| 28:DF:103:ILE:HD12 | 28:DF:104:THR:N    | 2.21                     | 0.56              |
| 29:DG:125:PRO:HG2  | 29:DG:129:GLU:HB2  | 1.88                     | 0.56              |
| 39:DR:6:GLN:HB3    | 39:DR:41:ILE:CD1   | 2.36                     | 0.56              |
| 41:DT:3:ARG:HB3    | 41:DT:5:GLU:CD     | 2.31                     | 0.56              |
| 43:DW:35:ILE:HB    | 43:DW:67:LYS:NZ    | 2.20                     | 0.56              |
| 1:AA:332:G:OP2     | 19:AT:2:ASN:HB3    | 2.06                     | 0.56              |
| 1:AA:529:G:H22     | 11:AL:47:ALA:CB    | 2.18                     | 0.56              |
| 1:AA:1329:A:OP1    | 12:AM:28:ARG:HB2   | 2.05                     | 0.56              |
| 13:AN:60:ARG:HE    | 13:AN:62:ARG:HE    | 1.53                     | 0.56              |
| 15:AP:20:VAL:HG22  | 15:AP:21:VAL:N     | 2.21                     | 0.56              |
| 23:BB:100:U:O3'    | 42:BU:90:LYS:HG2   | 2.06                     | 0.56              |
| 23:BB:198:C:C2'    | 23:BB:199:A:H5''   | 2.35                     | 0.56              |
| 23:BB:758:C:O2     | 23:BB:1981:A:H2    | 1.86                     | 0.56              |
| 23:BB:765:C:H2'    | 23:BB:766:U:C6     | 2.39                     | 0.56              |
| 23:BB:974:G:O4'    | 23:BB:990:A:N6     | 2.39                     | 0.56              |
| 23:BB:1739:A:H2'   | 23:BB:1740:G:C8    | 2.40                     | 0.56              |
| 23:BB:1923:U:H2'   | 23:BB:1924:C:C6    | 2.41                     | 0.56              |
| 23:BB:2239:G:H5'   | 25:BC:246:PRO:CG   | 2.35                     | 0.56              |
| 23:BB:2771:C:H2'   | 23:BB:2772:C:C6    | 2.41                     | 0.56              |
| 27:BE:149:ILE:CG1  | 27:BE:186:VAL:HG13 | 2.36                     | 0.56              |
| 29:BG:88:LEU:HD11  | 29:BG:95:ALA:HB2   | 1.88                     | 0.56              |
| 30:BH:128:HIS:CB   | 30:BH:144:VAL:HB   | 2.35                     | 0.56              |
| 32:BK:10:VAL:HG11  | 32:BK:15:GLY:O     | 2.04                     | 0.56              |
| 33:BL:110:VAL:HB   | 33:BL:126:ARG:CZ   | 2.35                     | 0.56              |
| 40:BS:27:LYS:H     | 40:BS:27:LYS:CD    | 2.11                     | 0.56              |
| 42:BU:6:ARG:C      | 42:BU:8:ASP:H      | 2.12                     | 0.56              |
| 44:BX:45:GLN:NE2   | 44:BX:45:GLN:N     | 2.53                     | 0.56              |
| 48:B1:42:VAL:HG12  | 48:B1:43:ARG:HE    | 1.71                     | 0.56              |
| 1:CA:93:U:C2'      | 1:CA:94:G:H5'      | 2.36                     | 0.56              |
| 1:CA:235:C:H2'     | 1:CA:236:A:H8      | 1.70                     | 0.56              |
| 1:CA:552:U:H2'     | 1:CA:553:A:C8      | 2.41                     | 0.56              |
| 1:CA:617:G:H5'     | 15:CP:46:LYS:HD3   | 1.87                     | 0.56              |
| 1:CA:1292:G:H2'    | 1:CA:1293:C:H6     | 1.71                     | 0.56              |
| 2:CC:35:ASP:O      | 2:CC:39:ARG:HG3    | 2.06                     | 0.56              |
| 3:CD:22:SER:H      | 3:CD:109:THR:CG2   | 2.19                     | 0.56              |
| 4:CE:55:VAL:N      | 4:CE:56:PRO:HD2    | 2.21                     | 0.56              |
| 4:CE:67:ARG:HB2    | 4:CE:67:ARG:NH1    | 2.20                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:CH:35:ILE:HG22   | 7:CH:39:LEU:HD23   | 1.88                     | 0.56              |
| 7:CH:100:ILE:HG13  | 7:CH:128:VAL:CG2   | 2.36                     | 0.56              |
| 13:CN:12:ARG:HG3   | 13:CN:53:ASP:O     | 2.05                     | 0.56              |
| 16:CQ:10:ARG:NH1   | 16:CQ:55:GLY:H     | 2.04                     | 0.56              |
| 18:CS:11:ASP:O     | 18:CS:14:LEU:HG    | 2.06                     | 0.56              |
| 23:DB:458:G:H22    | 23:DB:469:G:H2'    | 1.68                     | 0.56              |
| 23:DB:581:C:OP1    | 38:DQ:31:TYR:HB3   | 2.06                     | 0.56              |
| 23:DB:871:U:H2'    | 23:DB:872:U:H6     | 1.70                     | 0.56              |
| 23:DB:1082:U:N3    | 23:DB:1086:A:C2    | 2.73                     | 0.56              |
| 23:DB:1098:A:C3'   | 52:DI:3:LYS:HA     | 2.24                     | 0.56              |
| 23:DB:1438:U:N3    | 23:DB:1552:A:N6    | 2.53                     | 0.56              |
| 23:DB:1854:A:N6    | 23:DB:1888:G:H1'   | 2.21                     | 0.56              |
| 23:DB:1889:A:H2'   | 23:DB:1890:A:C8    | 2.41                     | 0.56              |
| 23:DB:2443:C:O2'   | 23:DB:2444:G:H5'   | 2.05                     | 0.56              |
| 23:DB:2771:C:H2'   | 23:DB:2772:C:C6    | 2.41                     | 0.56              |
| 25:DC:68:ARG:HD3   | 25:DC:103:ILE:HD12 | 1.88                     | 0.56              |
| 25:DC:145:MET:HG2  | 25:DC:152:GLN:HG2  | 1.88                     | 0.56              |
| 25:DC:171:VAL:HG12 | 25:DC:183:VAL:C    | 2.31                     | 0.56              |
| 26:DD:33:ARG:HB2   | 26:DD:33:ARG:NH1   | 2.18                     | 0.56              |
| 26:DD:50:VAL:HG11  | 26:DD:75:ALA:HB3   | 1.87                     | 0.56              |
| 27:DE:163:ASN:HB2  | 27:DE:167:VAL:O    | 2.05                     | 0.56              |
| 27:DE:191:ASP:O    | 27:DE:194:LYS:HG2  | 2.06                     | 0.56              |
| 29:DG:94:ARG:HB2   | 29:DG:105:SER:CB   | 2.35                     | 0.56              |
| 31:DJ:100:VAL:HG22 | 31:DJ:101:ILE:N    | 2.21                     | 0.56              |
| 33:DL:76:GLU:HA    | 33:DL:76:GLU:OE1   | 2.05                     | 0.56              |
| 36:DO:106:LEU:HD23 | 36:DO:106:LEU:C    | 2.31                     | 0.56              |
| 37:DP:59:THR:HG22  | 37:DP:74:GLN:HB3   | 1.88                     | 0.56              |
| 38:DQ:47:ARG:O     | 38:DQ:51:GLN:HG3   | 2.06                     | 0.56              |
| 39:DR:40:MET:O     | 39:DR:54:VAL:HG22  | 2.06                     | 0.56              |
| 45:DY:26:LEU:CD2   | 45:DY:46:MET:HE3   | 2.36                     | 0.56              |
| 47:D0:47:TYR:HB2   | 47:D0:50:GLY:O     | 2.06                     | 0.56              |
| 1:AA:69:G:H2'      | 1:AA:70:U:C6       | 2.40                     | 0.56              |
| 1:AA:97:G:H2'      | 1:AA:98:A:O4'      | 2.05                     | 0.56              |
| 1:AA:824:G:H2'     | 1:AA:825:A:H8      | 1.71                     | 0.56              |
| 1:AA:1090:U:H2'    | 1:AA:1091:U:C6     | 2.40                     | 0.56              |
| 6:AG:45:ALA:HB2    | 6:AG:116:ALA:O     | 2.05                     | 0.56              |
| 7:AH:111:THR:HG23  | 7:AH:114:ALA:HB2   | 1.87                     | 0.56              |
| 8:AI:18:VAL:HG21   | 8:AI:82:ILE:HG13   | 1.88                     | 0.56              |
| 8:AI:64:ILE:HD13   | 8:AI:78:ILE:HG21   | 1.87                     | 0.56              |
| 10:AK:12:ARG:HD2   | 10:AK:12:ARG:N     | 2.21                     | 0.56              |
| 17:AR:49:LYS:HA    | 17:AR:52:ARG:HD2   | 1.88                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:170:U:H2'    | 23:BB:171:U:H6     | 1.71                     | 0.56              |
| 23:BB:943:A:OP1    | 33:BL:42:SER:HB3   | 2.06                     | 0.56              |
| 23:BB:1460:U:H5''  | 23:BB:1461:C:C5    | 2.41                     | 0.56              |
| 23:BB:1862:G:O2'   | 23:BB:1863:G:H5'   | 2.06                     | 0.56              |
| 23:BB:2825:G:H2'   | 23:BB:2826:A:H5'   | 1.88                     | 0.56              |
| 27:BE:122:GLU:HB3  | 27:BE:152:GLU:CB   | 2.35                     | 0.56              |
| 29:BG:159:LYS:O    | 29:BG:159:LYS:HG3  | 2.05                     | 0.56              |
| 31:BJ:10:THR:HG22  | 31:BJ:50:THR:CA    | 2.35                     | 0.56              |
| 31:BJ:35:ARG:HH21  | 31:BJ:40:HIS:N     | 2.04                     | 0.56              |
| 34:BM:108:VAL:N    | 34:BM:109:PRO:CD   | 2.69                     | 0.56              |
| 38:BQ:34:ALA:C     | 38:BQ:38:VAL:HG12  | 2.31                     | 0.56              |
| 40:BS:7:HIS:CG     | 40:BS:8:ARG:H      | 2.23                     | 0.56              |
| 42:BU:23:LYS:NZ    | 42:BU:24:VAL:HG22  | 2.21                     | 0.56              |
| 43:BW:6:GLY:C      | 43:BW:8:SER:H      | 2.14                     | 0.56              |
| 43:BW:42:THR:CB    | 43:BW:66:VAL:H     | 2.19                     | 0.56              |
| 43:BW:47:GLY:N     | 43:BW:67:LYS:HZ3   | 2.04                     | 0.56              |
| 46:BZ:15:SER:HB2   | 46:BZ:25:ARG:HH12  | 1.71                     | 0.56              |
| 46:BZ:48:GLN:H     | 46:BZ:51:VAL:HB    | 1.69                     | 0.56              |
| 48:B1:31:GLU:HB3   | 48:B1:32:LYS:HE3   | 1.86                     | 0.56              |
| 1:CA:272:C:H2'     | 1:CA:273:U:H6      | 1.70                     | 0.56              |
| 1:CA:875:U:O2'     | 7:CH:14:ARG:HD2    | 2.05                     | 0.56              |
| 1:CA:923:A:OP1     | 4:CE:25:LYS:HB3    | 2.05                     | 0.56              |
| 1:CA:948:C:O2'     | 1:CA:949:A:H5'     | 2.05                     | 0.56              |
| 1:CA:1002:G:H2'    | 1:CA:1003:G:O4'    | 2.06                     | 0.56              |
| 1:CA:1063:C:H3'    | 1:CA:1064:G:H2'    | 1.87                     | 0.56              |
| 3:CD:151:GLN:NE2   | 3:CD:153:ARG:HD2   | 2.20                     | 0.56              |
| 12:CM:78:ARG:NH1   | 12:CM:79:LEU:HD23  | 2.19                     | 0.56              |
| 13:CN:42:ASN:HB3   | 13:CN:46:LYS:HE2   | 1.86                     | 0.56              |
| 18:CS:62:THR:HG21  | 18:CS:64:GLU:OE1   | 2.05                     | 0.56              |
| 20:CB:31:PHE:HB2   | 20:CB:41:ASN:HA    | 1.88                     | 0.56              |
| 23:DB:324:A:H2'    | 23:DB:325:G:O4'    | 2.06                     | 0.56              |
| 23:DB:621:A:H2'    | 23:DB:622:G:O4'    | 2.06                     | 0.56              |
| 23:DB:675:A:OP1    | 27:DE:58:LYS:HE2   | 2.06                     | 0.56              |
| 23:DB:703:U:H2'    | 23:DB:704:G:O4'    | 2.05                     | 0.56              |
| 23:DB:1459:G:C2'   | 23:DB:1460:U:H5'   | 2.35                     | 0.56              |
| 23:DB:2562:U:H1'   | 32:DK:23:LYS:HE2   | 1.88                     | 0.56              |
| 23:DB:2665:A:O2'   | 23:DB:2666:C:H5'   | 2.05                     | 0.56              |
| 23:DB:2888:C:H2'   | 23:DB:2889:C:H6    | 1.69                     | 0.56              |
| 24:DV:6:ALA:O      | 24:DV:65:VAL:HA    | 2.06                     | 0.56              |
| 26:DD:146:ILE:CD1  | 26:DD:155:VAL:HG13 | 2.36                     | 0.56              |
| 28:DF:107:VAL:HG12 | 28:DF:108:PRO:CD   | 2.32                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:DJ:98:GLU:CD   | 31:DJ:98:GLU:H    | 2.12                     | 0.56              |
| 35:DN:72:ASP:OD1  | 35:DN:74:GLU:HB3  | 2.05                     | 0.56              |
| 35:DN:87:PHE:HB2  | 35:DN:94:TYR:CE2  | 2.40                     | 0.56              |
| 43:DW:42:THR:N    | 43:DW:65:LYS:HA   | 2.20                     | 0.56              |
| 44:DX:25:GLN:HG2  | 44:DX:26:PHE:N    | 2.20                     | 0.56              |
| 49:D2:37:LYS:HD3  | 49:D2:37:LYS:C    | 2.31                     | 0.56              |
| 1:AA:129:A:H1'    | 1:AA:130:A:C8     | 2.41                     | 0.56              |
| 1:AA:266:G:O2'    | 1:AA:267:C:H3'    | 2.06                     | 0.56              |
| 1:AA:1422:G:OP1   | 32:BK:48:PRO:HA   | 2.06                     | 0.56              |
| 4:AE:104:ILE:HG23 | 4:AE:111:ARG:NH1  | 2.21                     | 0.56              |
| 6:AG:24:LYS:O     | 6:AG:28:ILE:HG13  | 2.06                     | 0.56              |
| 6:AG:61:PHE:O     | 6:AG:65:LEU:HD13  | 2.06                     | 0.56              |
| 7:AH:65:PHE:CD2   | 7:AH:66:GLN:HG3   | 2.41                     | 0.56              |
| 18:AS:68:HIS:NE2  | 18:AS:72:GLU:HG3  | 2.21                     | 0.56              |
| 23:BB:140:C:H4'   | 23:BB:141:G:H21   | 1.71                     | 0.56              |
| 23:BB:315:G:H2'   | 23:BB:316:C:C6    | 2.41                     | 0.56              |
| 23:BB:527:C:H5''  | 23:BB:2779:U:C2   | 2.41                     | 0.56              |
| 23:BB:581:C:H2'   | 23:BB:582:A:H8    | 1.70                     | 0.56              |
| 23:BB:639:U:H2'   | 23:BB:640:C:H6    | 1.69                     | 0.56              |
| 23:BB:663:G:OP1   | 33:BL:27:LEU:HD21 | 2.06                     | 0.56              |
| 23:BB:996:A:O3'   | 38:BQ:92:LYS:HE2  | 2.06                     | 0.56              |
| 23:BB:1064:C:H4'  | 52:BI:90:GLY:HA2  | 1.88                     | 0.56              |
| 23:BB:1080:A:H2'  | 23:BB:1081:U:H6   | 1.71                     | 0.56              |
| 23:BB:1316:U:O2'  | 23:BB:1317:G:H5'  | 2.05                     | 0.56              |
| 23:BB:1534:U:H2'  | 23:BB:1536:C:N3   | 2.21                     | 0.56              |
| 23:BB:1550:C:H2'  | 23:BB:1551:A:C8   | 2.40                     | 0.56              |
| 23:BB:1656:C:P    | 26:BD:141:ARG:HD3 | 2.45                     | 0.56              |
| 23:BB:1710:G:H4'  | 23:BB:2858:C:O2   | 2.06                     | 0.56              |
| 23:BB:2484:G:OP1  | 34:BM:44:ARG:HD2  | 2.06                     | 0.56              |
| 23:BB:2626:C:O2'  | 23:BB:2627:G:H5'  | 2.06                     | 0.56              |
| 32:BK:40:LYS:HE3  | 32:BK:57:VAL:HG12 | 1.88                     | 0.56              |
| 33:BL:63:LYS:HA   | 50:B3:24:LYS:HD3  | 1.87                     | 0.56              |
| 34:BM:3:GLN:OE1   | 34:BM:47:GLU:HB2  | 2.05                     | 0.56              |
| 34:BM:53:MET:O    | 34:BM:54:THR:HG23 | 2.06                     | 0.56              |
| 37:BP:29:VAL:CG2  | 37:BP:47:ILE:HD11 | 2.36                     | 0.56              |
| 37:BP:80:VAL:O    | 37:BP:80:VAL:HG13 | 2.05                     | 0.56              |
| 43:BW:65:LYS:HE2  | 43:BW:65:LYS:C    | 2.31                     | 0.56              |
| 47:B0:16:ARG:HA   | 47:B0:19:ASP:OD2  | 2.05                     | 0.56              |
| 50:B3:53:ASP:O    | 50:B3:56:LEU:HB3  | 2.06                     | 0.56              |
| 1:CA:426:U:H2'    | 1:CA:427:U:C6     | 2.41                     | 0.56              |
| 1:CA:576:C:OP2    | 1:CA:576:C:H3'    | 2.06                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:673:A:H1'    | 17:CR:63:TYR:CE1  | 2.40                     | 0.56              |
| 1:CA:676:A:H5''   | 10:CK:114:PRO:HB2 | 1.87                     | 0.56              |
| 1:CA:1151:A:O2'   | 1:CA:1152:A:H8    | 1.89                     | 0.56              |
| 1:CA:1234:C:H1'   | 1:CA:1364:U:O2    | 2.06                     | 0.56              |
| 11:CL:30:ARG:O    | 11:CL:56:LEU:HA   | 2.06                     | 0.56              |
| 12:CM:3:ILE:HA    | 12:CM:56:ARG:NH1  | 2.21                     | 0.56              |
| 16:CQ:24:ILE:HD12 | 16:CQ:24:ILE:N    | 2.21                     | 0.56              |
| 18:CS:15:LEU:HA   | 18:CS:18:VAL:CG1  | 2.34                     | 0.56              |
| 19:CT:61:ALA:HA   | 19:CT:67:HIS:N    | 2.17                     | 0.56              |
| 23:DB:30:G:H2'    | 23:DB:31:C:H6     | 1.71                     | 0.56              |
| 23:DB:566:U:O2'   | 23:DB:567:U:H5'   | 2.06                     | 0.56              |
| 23:DB:581:C:H2'   | 23:DB:582:A:H8    | 1.70                     | 0.56              |
| 23:DB:1360:G:C2'  | 23:DB:1361:G:H5'  | 2.36                     | 0.56              |
| 23:DB:1534:U:H2'  | 23:DB:1536:C:N3   | 2.21                     | 0.56              |
| 23:DB:1666:G:O3'  | 32:DK:6:THR:HG23  | 2.06                     | 0.56              |
| 23:DB:2074:U:H2'  | 23:DB:2075:U:C6   | 2.41                     | 0.56              |
| 23:DB:2091:C:H5'  | 46:DZ:49:ARG:HG3  | 1.88                     | 0.56              |
| 23:DB:2636:C:C5'  | 26:DD:80:TRP:HE1  | 2.19                     | 0.56              |
| 25:DC:63:ILE:HG22 | 25:DC:64:VAL:N    | 2.21                     | 0.56              |
| 28:DF:16:MET:O    | 28:DF:20:ASN:HA   | 2.06                     | 0.56              |
| 28:DF:107:VAL:N   | 28:DF:108:PRO:CD  | 2.69                     | 0.56              |
| 33:DL:90:VAL:HG13 | 33:DL:90:VAL:O    | 2.06                     | 0.56              |
| 39:DR:79:ARG:HD2  | 39:DR:80:ARG:N    | 2.21                     | 0.56              |
| 42:DU:25:LYS:HA   | 42:DU:34:ILE:H    | 1.71                     | 0.56              |
| 43:DW:21:GLY:HA3  | 43:DW:32:ALA:HA   | 1.86                     | 0.56              |
| 46:DZ:11:GLU:H    | 46:DZ:27:THR:HG22 | 1.71                     | 0.56              |
| 48:D1:7:LYS:HB3   | 48:D1:24:LYS:NZ   | 2.21                     | 0.56              |
| 48:D1:9:LYS:HA    | 48:D1:24:LYS:CB   | 2.36                     | 0.56              |
| 50:D3:12:ARG:O    | 50:D3:13:PHE:HB2  | 2.06                     | 0.56              |
| 1:AA:272:C:H2'    | 1:AA:273:U:H6     | 1.71                     | 0.55              |
| 1:AA:383:A:H2'    | 1:AA:384:G:O4'    | 2.05                     | 0.55              |
| 1:AA:450:G:H4'    | 15:AP:41:PRO:HB2  | 1.87                     | 0.55              |
| 1:AA:958:A:N1     | 18:AS:53:GLY:HA3  | 2.21                     | 0.55              |
| 1:AA:1404:C:H2'   | 1:AA:1405:G:C8    | 2.41                     | 0.55              |
| 2:AC:181:ILE:HD12 | 2:AC:181:ILE:N    | 2.20                     | 0.55              |
| 3:AD:58:GLN:OE1   | 3:AD:62:ARG:HG3   | 2.07                     | 0.55              |
| 6:AG:72:VAL:HA    | 6:AG:89:GLU:HA    | 1.86                     | 0.55              |
| 16:AQ:4:ILE:CD1   | 16:AQ:5:ARG:H     | 2.20                     | 0.55              |
| 16:AQ:8:GLN:HB3   | 16:AQ:57:VAL:HG13 | 1.88                     | 0.55              |
| 19:AT:62:ALA:O    | 19:AT:63:LYS:HG3  | 2.05                     | 0.55              |
| 20:AB:125:PHE:HD2 | 20:AB:125:PHE:H   | 1.53                     | 0.55              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:BB:419:U:H2'    | 23:BB:420:C:C6    | 2.41                     | 0.55              |
| 23:BB:543:G:C3'    | 23:BB:544:C:H5''  | 2.36                     | 0.55              |
| 23:BB:1168:G:H2'   | 23:BB:1169:A:O4'  | 2.06                     | 0.55              |
| 23:BB:1241:A:C2'   | 23:BB:1242:U:H5'  | 2.36                     | 0.55              |
| 23:BB:2053:G:O2'   | 23:BB:2054:A:H5'  | 2.06                     | 0.55              |
| 24:BV:21:ARG:NH2   | 24:BV:27:PRO:HG3  | 2.21                     | 0.55              |
| 28:BF:121:PHE:HE2  | 28:BF:166:ARG:H   | 1.54                     | 0.55              |
| 35:BN:9:GLN:HB2    | 35:BN:17:ARG:CZ   | 2.36                     | 0.55              |
| 38:BQ:3:VAL:HG12   | 38:BQ:5:ARG:HG3   | 1.87                     | 0.55              |
| 39:BR:4:VAL:HG22   | 39:BR:5:PHE:H     | 1.71                     | 0.55              |
| 39:BR:5:PHE:HA     | 39:BR:40:MET:HG3  | 1.86                     | 0.55              |
| 42:BU:2:ALA:C      | 42:BU:3:LYS:HD3   | 2.31                     | 0.55              |
| 46:BZ:30:HIS:H     | 46:BZ:48:GLN:CD   | 2.13                     | 0.55              |
| 1:CA:301:G:H2'     | 1:CA:302:G:H8     | 1.71                     | 0.55              |
| 1:CA:1014:A:C2     | 1:CA:1219:A:H1'   | 2.41                     | 0.55              |
| 23:DB:245:G:O2'    | 23:DB:246:C:H5'   | 2.07                     | 0.55              |
| 23:DB:1460:U:H5''  | 23:DB:1461:C:C5   | 2.41                     | 0.55              |
| 23:DB:1938:A:O2'   | 23:DB:1939:U:H5'' | 2.06                     | 0.55              |
| 23:DB:2538:C:O2'   | 23:DB:2539:C:H5'  | 2.06                     | 0.55              |
| 25:DC:153:LEU:HD23 | 25:DC:153:LEU:H   | 1.71                     | 0.55              |
| 26:DD:11:MET:O     | 26:DD:22:ILE:HA   | 2.06                     | 0.55              |
| 27:DE:48:THR:HG23  | 27:DE:84:THR:HA   | 1.88                     | 0.55              |
| 32:DK:64:ARG:N     | 32:DK:83:ALA:HB3  | 2.22                     | 0.55              |
| 35:DN:26:GLY:HA2   | 35:DN:75:ILE:HD13 | 1.87                     | 0.55              |
| 36:DO:49:VAL:HG22  | 36:DO:50:ALA:N    | 2.21                     | 0.55              |
| 39:DR:42:ALA:HB1   | 39:DR:53:PHE:CD1  | 2.40                     | 0.55              |
| 52:DI:2:LYS:HB3    | 52:DI:2:LYS:NZ    | 2.21                     | 0.55              |
| 1:AA:9:G:H5'       | 4:AE:107:GLY:HA3  | 1.86                     | 0.55              |
| 1:AA:196:A:O5'     | 19:AT:63:LYS:HE2  | 2.05                     | 0.55              |
| 1:AA:235:C:H2'     | 1:AA:236:A:H8     | 1.70                     | 0.55              |
| 1:AA:720:C:H5''    | 17:AR:40:PRO:HA   | 1.87                     | 0.55              |
| 1:AA:983:A:H5'     | 1:AA:984:C:OP2    | 2.06                     | 0.55              |
| 1:AA:1202:U:H2'    | 1:AA:1203:C:H5'   | 1.87                     | 0.55              |
| 1:AA:1397:C:H4'    | 1:AA:1398:A:OP2   | 2.04                     | 0.55              |
| 4:AE:81:GLN:HE21   | 4:AE:147:ASN:C    | 2.14                     | 0.55              |
| 8:AI:30:ASN:HD21   | 8:AI:65:THR:HA    | 1.71                     | 0.55              |
| 10:AK:85:VAL:HG21  | 10:AK:96:ILE:HD11 | 1.88                     | 0.55              |
| 11:AL:48:LEU:H     | 11:AL:48:LEU:CD2  | 2.13                     | 0.55              |
| 12:AM:11:HIS:O     | 12:AM:12:LYS:HG2  | 2.06                     | 0.55              |
| 18:AS:32:THR:HB    | 18:AS:49:ALA:O    | 2.05                     | 0.55              |
| 19:AT:74:HIS:O     | 19:AT:78:LEU:HD12 | 2.05                     | 0.55              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:442:G:H22    | 27:BE:46:GLN:NE2   | 2.03                     | 0.55              |
| 23:BB:533:G:H2'    | 23:BB:534:U:C6     | 2.40                     | 0.55              |
| 23:BB:1244:A:O2'   | 23:BB:1245:G:H5'   | 2.05                     | 0.55              |
| 23:BB:2398:U:H2'   | 23:BB:2399:G:H8    | 1.71                     | 0.55              |
| 23:BB:2538:C:O2'   | 23:BB:2539:C:H5'   | 2.06                     | 0.55              |
| 23:BB:2600:A:O2'   | 23:BB:2601:C:H5'   | 2.05                     | 0.55              |
| 25:BC:130:PRO:HB2  | 25:BC:133:ASN:ND2  | 2.21                     | 0.55              |
| 25:BC:209:ALA:HA   | 25:BC:213:ARG:NE   | 2.21                     | 0.55              |
| 26:BD:122:VAL:HG22 | 26:BD:128:ARG:HB2  | 1.89                     | 0.55              |
| 29:BG:71:LEU:HA    | 29:BG:74:MET:CG    | 2.36                     | 0.55              |
| 36:BO:18:LEU:C     | 36:BO:18:LEU:HD12  | 2.31                     | 0.55              |
| 37:BP:83:ILE:HB    | 37:BP:85:VAL:HG23  | 1.88                     | 0.55              |
| 37:BP:88:ARG:HA    | 37:BP:88:ARG:HE    | 1.70                     | 0.55              |
| 39:BR:53:PHE:CG    | 39:BR:54:VAL:N     | 2.73                     | 0.55              |
| 47:B0:12:ARG:C     | 47:B0:12:ARG:HD3   | 2.31                     | 0.55              |
| 1:CA:21:G:H2'      | 1:CA:22:G:C8       | 2.40                     | 0.55              |
| 1:CA:123:U:OP1     | 1:CA:312:C:H5'     | 2.07                     | 0.55              |
| 1:CA:922:G:N3      | 1:CA:1398:A:H2     | 2.05                     | 0.55              |
| 1:CA:1226:C:H4'    | 1:CA:1227:A:OP1    | 2.05                     | 0.55              |
| 1:CA:1348:U:H4'    | 8:CI:121:ARG:HG3   | 1.88                     | 0.55              |
| 1:CA:1509:C:O2'    | 1:CA:1510:C:H5'    | 2.05                     | 0.55              |
| 3:CD:55:ARG:HH11   | 3:CD:55:ARG:HG3    | 1.71                     | 0.55              |
| 10:CK:81:LEU:HD23  | 10:CK:99:LEU:HD21  | 1.87                     | 0.55              |
| 13:CN:56:PRO:O     | 13:CN:59:GLN:HG3   | 2.05                     | 0.55              |
| 23:DB:918:A:C2'    | 23:DB:919:U:H5'    | 2.30                     | 0.55              |
| 23:DB:1559:U:H3'   | 23:DB:1560:G:H5'   | 1.88                     | 0.55              |
| 23:DB:1657:U:OP2   | 26:DD:141:ARG:HG3  | 2.07                     | 0.55              |
| 23:DB:1923:U:H2'   | 23:DB:1924:C:C6    | 2.41                     | 0.55              |
| 23:DB:2467:C:O4'   | 34:DM:118:LYS:HD2  | 2.07                     | 0.55              |
| 23:DB:2586:U:H2'   | 23:DB:2587:A:C8    | 2.41                     | 0.55              |
| 25:DC:67:LYS:HG2   | 25:DC:149:LYS:O    | 2.05                     | 0.55              |
| 25:DC:193:GLU:C    | 25:DC:194:VAL:HG22 | 2.30                     | 0.55              |
| 30:DH:80:ILE:HD12  | 30:DH:80:ILE:N     | 2.21                     | 0.55              |
| 33:DL:124:GLY:C    | 33:DL:125:LEU:HD23 | 2.32                     | 0.55              |
| 34:DM:41:LEU:HB2   | 34:DM:95:LEU:HD22  | 1.87                     | 0.55              |
| 34:DM:114:ARG:O    | 34:DM:117:PHE:HD1  | 1.89                     | 0.55              |
| 37:DP:1:SER:HB2    | 37:DP:5:LYS:HG2    | 1.88                     | 0.55              |
| 50:D3:12:ARG:CB    | 50:D3:23:HIS:HB2   | 2.31                     | 0.55              |
| 1:AA:366:A:O2'     | 1:AA:367:U:OP1     | 2.24                     | 0.55              |
| 1:AA:1241:G:H2'    | 1:AA:1242:G:C8     | 2.38                     | 0.55              |
| 1:AA:1308:U:OP1    | 12:AM:95:PRO:HA    | 2.07                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:AM:15:VAL:CG2   | 12:AM:33:LEU:HD12  | 2.35                     | 0.55              |
| 15:AP:23:ASP:O     | 15:AP:26:ASN:HB2   | 2.06                     | 0.55              |
| 23:BB:214:G:H2'    | 23:BB:215:G:C8     | 2.41                     | 0.55              |
| 23:BB:650:C:H5''   | 50:B3:22:LYS:HZ3   | 1.71                     | 0.55              |
| 23:BB:729:G:H4'    | 23:BB:763:G:C5'    | 2.36                     | 0.55              |
| 23:BB:1199:U:H2'   | 23:BB:1200:C:C6    | 2.41                     | 0.55              |
| 23:BB:1291:C:O2'   | 23:BB:1292:G:H5'   | 2.07                     | 0.55              |
| 23:BB:1381:G:H2'   | 23:BB:1382:G:H5'   | 1.86                     | 0.55              |
| 23:BB:2143:C:O3'   | 23:BB:2144:G:H4'   | 2.06                     | 0.55              |
| 23:BB:2400:G:O2'   | 23:BB:2401:U:H5'   | 2.07                     | 0.55              |
| 25:BC:179:GLU:HG3  | 25:BC:266:ILE:HG22 | 1.87                     | 0.55              |
| 27:BE:147:LEU:HD13 | 27:BE:182:ALA:O    | 2.07                     | 0.55              |
| 27:BE:187:VAL:HG23 | 27:BE:187:VAL:O    | 2.06                     | 0.55              |
| 28:BF:33:ILE:HA    | 28:BF:155:ILE:HA   | 1.88                     | 0.55              |
| 30:BH:4:ILE:H      | 30:BH:37:VAL:CB    | 2.17                     | 0.55              |
| 32:BK:47:ILE:HG23  | 32:BK:48:PRO:HD2   | 1.87                     | 0.55              |
| 33:BL:63:LYS:CG    | 50:B3:11:LYS:HA    | 2.37                     | 0.55              |
| 38:BQ:88:GLU:HA    | 39:BR:53:PHE:CD2   | 2.41                     | 0.55              |
| 43:BW:56:HIS:CE1   | 43:BW:58:LEU:HB2   | 2.41                     | 0.55              |
| 44:BX:7:ARG:NH1    | 44:BX:7:ARG:HA     | 2.21                     | 0.55              |
| 45:BY:6:ILE:HD13   | 45:BY:35:VAL:O     | 2.06                     | 0.55              |
| 49:B2:34:ARG:NE    | 49:B2:42:LEU:HD13  | 2.21                     | 0.55              |
| 1:CA:220:G:O2'     | 1:CA:221:C:H5'     | 2.06                     | 0.55              |
| 1:CA:449:G:H2'     | 1:CA:450:G:C8      | 2.40                     | 0.55              |
| 1:CA:1217:C:H2'    | 1:CA:1218:C:H6     | 1.71                     | 0.55              |
| 5:CF:86:ARG:HD3    | 17:CR:63:TYR:O     | 2.06                     | 0.55              |
| 19:CT:73:ARG:HG3   | 19:CT:74:HIS:N     | 2.21                     | 0.55              |
| 20:CB:209:VAL:O    | 20:CB:213:LEU:HD12 | 2.05                     | 0.55              |
| 23:DB:192:C:H2'    | 23:DB:193:U:H5'    | 1.88                     | 0.55              |
| 23:DB:1022:G:H8    | 31:DJ:68:LYS:HE3   | 1.69                     | 0.55              |
| 23:DB:1098:A:C3'   | 52:DI:3:LYS:HB3    | 2.36                     | 0.55              |
| 23:DB:2103:C:H2'   | 23:DB:2104:C:O4'   | 2.07                     | 0.55              |
| 26:DD:56:LYS:NZ    | 26:DD:56:LYS:HB3   | 2.21                     | 0.55              |
| 26:DD:114:LYS:HB2  | 26:DD:114:LYS:HZ2  | 1.71                     | 0.55              |
| 27:DE:45:ALA:O     | 27:DE:46:GLN:HB3   | 2.05                     | 0.55              |
| 27:DE:147:LEU:C    | 27:DE:148:ILE:HG23 | 2.31                     | 0.55              |
| 34:DM:15:GLY:C     | 34:DM:16:ARG:HG3   | 2.31                     | 0.55              |
| 35:DN:66:ALA:O     | 35:DN:70:THR:HB    | 2.06                     | 0.55              |
| 36:DO:26:LEU:O     | 36:DO:27:VAL:HG13  | 2.06                     | 0.55              |
| 36:DO:67:ASN:HD22  | 36:DO:68:LYS:N     | 2.04                     | 0.55              |
| 37:DP:29:VAL:O     | 37:DP:31:VAL:HG23  | 2.06                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 52:DI:79:LEU:HD11 | 52:DI:131:THR:OG1 | 2.06                     | 0.55              |
| 1:AA:34:C:H2'     | 1:AA:35:G:C8      | 2.41                     | 0.55              |
| 1:AA:462:G:H3'    | 1:AA:463:U:H5''   | 1.88                     | 0.55              |
| 1:AA:981:U:H4'    | 13:AN:60:ARG:HG3  | 1.88                     | 0.55              |
| 1:AA:1320:C:H41   | 18:AS:36:ARG:HG2  | 1.71                     | 0.55              |
| 1:AA:1369:C:H2'   | 1:AA:1370:G:C8    | 2.42                     | 0.55              |
| 5:AF:64:VAL:CG1   | 5:AF:65:GLU:H     | 2.13                     | 0.55              |
| 6:AG:41:ILE:HD11  | 6:AG:116:ALA:HB2  | 1.88                     | 0.55              |
| 8:AI:38:PHE:C     | 8:AI:44:ARG:HG2   | 2.31                     | 0.55              |
| 13:AN:9:GLU:O     | 13:AN:13:VAL:HG23 | 2.07                     | 0.55              |
| 23:BB:78:U:H2'    | 23:BB:79:C:H6     | 1.70                     | 0.55              |
| 23:BB:84:A:O5'    | 42:BU:91:LYS:HD3  | 2.07                     | 0.55              |
| 23:BB:295:G:O2'   | 23:BB:296:U:H5'   | 2.07                     | 0.55              |
| 23:BB:397:U:OP1   | 46:BZ:29:GLY:HA2  | 2.07                     | 0.55              |
| 23:BB:621:A:H2'   | 23:BB:622:G:O4'   | 2.06                     | 0.55              |
| 23:BB:667:U:H2'   | 23:BB:668:A:O4'   | 2.07                     | 0.55              |
| 23:BB:1113:U:H5'' | 29:BG:2:ARG:N     | 2.22                     | 0.55              |
| 23:BB:1444:G:H2'  | 23:BB:1445:G:C8   | 2.40                     | 0.55              |
| 23:BB:1854:A:N6   | 23:BB:1888:G:H1'  | 2.21                     | 0.55              |
| 23:BB:2657:A:H2'  | 23:BB:2658:C:O4'  | 2.07                     | 0.55              |
| 23:BB:2729:G:H2'  | 23:BB:2730:C:H6   | 1.71                     | 0.55              |
| 23:BB:2888:C:H2'  | 23:BB:2889:C:H6   | 1.70                     | 0.55              |
| 28:BF:15:LEU:HA   | 28:BF:18:GLU:HB3  | 1.88                     | 0.55              |
| 30:BH:48:GLU:C    | 30:BH:50:ARG:H    | 2.15                     | 0.55              |
| 37:BP:24:THR:HG21 | 37:BP:111:GLU:HG2 | 1.88                     | 0.55              |
| 40:BS:17:VAL:HG23 | 40:BS:76:VAL:HG11 | 1.88                     | 0.55              |
| 42:BU:23:LYS:O    | 42:BU:25:LYS:N    | 2.40                     | 0.55              |
| 42:BU:78:LYS:CE   | 42:BU:96:LYS:HB2  | 2.37                     | 0.55              |
| 4:CE:65:LYS:NZ    | 4:CE:65:LYS:HB3   | 2.21                     | 0.55              |
| 4:CE:104:ILE:C    | 4:CE:104:ILE:HD13 | 2.31                     | 0.55              |
| 6:CG:91:ARG:HB3   | 6:CG:92:PRO:HD2   | 1.88                     | 0.55              |
| 9:CJ:36:VAL:HA    | 9:CJ:76:ILE:CG2   | 2.37                     | 0.55              |
| 17:CR:72:ARG:HB2  | 17:CR:72:ARG:CZ   | 2.36                     | 0.55              |
| 23:DB:78:U:H2'    | 23:DB:79:C:C6     | 2.41                     | 0.55              |
| 23:DB:935:C:H2'   | 23:DB:936:A:H8    | 1.71                     | 0.55              |
| 23:DB:1099:G:OP2  | 52:DI:2:LYS:O     | 2.23                     | 0.55              |
| 23:DB:1197:G:H2'  | 23:DB:1198:U:C6   | 2.41                     | 0.55              |
| 23:DB:1251:C:O2'  | 23:DB:1252:G:H3'  | 2.07                     | 0.55              |
| 23:DB:1550:C:H2'  | 23:DB:1551:A:C8   | 2.41                     | 0.55              |
| 23:DB:1551:A:H3'  | 23:DB:1552:A:H5'' | 1.87                     | 0.55              |
| 23:DB:2250:G:H21  | 23:DB:2496:C:H4'  | 1.71                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DB:2398:U:H2'  | 23:DB:2399:G:H8   | 1.70                     | 0.55              |
| 23:DB:2839:G:H2'  | 23:DB:2840:C:C6   | 2.41                     | 0.55              |
| 25:DC:33:LEU:CD2  | 25:DC:34:GLU:HG3  | 2.25                     | 0.55              |
| 26:DD:4:LEU:HD23  | 26:DD:77:ARG:HD3  | 1.88                     | 0.55              |
| 26:DD:127:PHE:C   | 26:DD:128:ARG:HD3 | 2.31                     | 0.55              |
| 27:DE:59:PRO:HB2  | 27:DE:60:TRP:CD1  | 2.41                     | 0.55              |
| 30:DH:3:VAL:HB    | 30:DH:37:VAL:HG11 | 1.87                     | 0.55              |
| 34:DM:2:LEU:HB2   | 34:DM:47:GLU:HG2  | 1.88                     | 0.55              |
| 37:DP:23:ASP:HB2  | 37:DP:93:LYS:HE2  | 1.89                     | 0.55              |
| 37:DP:86:LYS:HE3  | 37:DP:88:ARG:HB2  | 1.89                     | 0.55              |
| 39:DR:63:VAL:CG2  | 39:DR:64:VAL:H    | 2.09                     | 0.55              |
| 40:DS:45:VAL:C    | 40:DS:47:VAL:H    | 2.14                     | 0.55              |
| 41:DT:66:LYS:HZ3  | 41:DT:66:LYS:C    | 2.15                     | 0.55              |
| 42:DU:28:LEU:HD21 | 42:DU:31:GLY:HA3  | 1.89                     | 0.55              |
| 43:DW:23:LYS:HD3  | 43:DW:24:ARG:HD2  | 1.88                     | 0.55              |
| 43:DW:35:ILE:HD12 | 43:DW:35:ILE:N    | 2.14                     | 0.55              |
| 45:DY:36:GLU:O    | 45:DY:37:ARG:HG2  | 2.06                     | 0.55              |
| 47:D0:26:SER:HB2  | 47:D0:38:LEU:CD2  | 2.37                     | 0.55              |
| 48:D1:22:THR:HG21 | 50:D3:34:LYS:NZ   | 2.21                     | 0.55              |
| 1:AA:19:A:OP1     | 4:AE:134:ASN:ND2  | 2.39                     | 0.55              |
| 1:AA:87:C:H2'     | 1:AA:88:U:C4'     | 2.36                     | 0.55              |
| 1:AA:335:C:H2'    | 1:AA:336:A:H8     | 1.72                     | 0.55              |
| 1:AA:1435:G:H2'   | 1:AA:1436:U:C6    | 2.41                     | 0.55              |
| 4:AE:13:LYS:HD2   | 4:AE:112:ALA:HB1  | 1.89                     | 0.55              |
| 15:AP:1:MET:N     | 15:AP:24:SER:HB3  | 2.22                     | 0.55              |
| 23:BB:338:G:C2    | 23:BB:339:U:H1'   | 2.41                     | 0.55              |
| 23:BB:363:G:H2'   | 23:BB:364:C:C6    | 2.42                     | 0.55              |
| 23:BB:654:A:H2'   | 23:BB:655:A:C5'   | 2.33                     | 0.55              |
| 23:BB:1360:G:C2'  | 23:BB:1361:G:H5'  | 2.37                     | 0.55              |
| 23:BB:1564:C:O2'  | 23:BB:1565:C:H5'  | 2.06                     | 0.55              |
| 23:BB:2639:A:H2'  | 23:BB:2640:G:O4'  | 2.06                     | 0.55              |
| 23:BB:2848:G:O2'  | 37:BP:96:LEU:HD22 | 2.06                     | 0.55              |
| 23:BB:2849:U:H4'  | 23:BB:2850:A:C5'  | 2.37                     | 0.55              |
| 24:BV:2:PHE:O     | 24:BV:3:THR:HG23  | 2.07                     | 0.55              |
| 25:BC:254:LYS:HD2 | 25:BC:254:LYS:N   | 2.22                     | 0.55              |
| 27:BE:48:THR:HG23 | 27:BE:87:ALA:H    | 1.72                     | 0.55              |
| 28:BF:174:PHE:N   | 28:BF:175:PRO:HD2 | 2.22                     | 0.55              |
| 29:BG:5:LYS:HB3   | 29:BG:68:ARG:CZ   | 2.36                     | 0.55              |
| 33:BL:30:THR:HG22 | 33:BL:36:LYS:HZ1  | 1.72                     | 0.55              |
| 38:BQ:5:ARG:HH11  | 38:BQ:5:ARG:CB    | 2.13                     | 0.55              |
| 40:BS:29:VAL:HG11 | 40:BS:69:LEU:HB2  | 1.88                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:BT:35:ALA:O    | 41:BT:81:LYS:HD3  | 2.06                     | 0.55              |
| 46:BZ:33:ASN:CB   | 46:BZ:44:PHE:HB2  | 2.29                     | 0.55              |
| 47:B0:9:ARG:NH1   | 47:B0:9:ARG:HB3   | 2.22                     | 0.55              |
| 49:B2:35:ARG:O    | 49:B2:39:ARG:HA   | 2.06                     | 0.55              |
| 1:CA:214:C:H2'    | 1:CA:215:C:H6     | 1.72                     | 0.55              |
| 1:CA:279:A:H4'    | 1:CA:280:C:OP2    | 2.07                     | 0.55              |
| 1:CA:399:G:H2'    | 1:CA:400:C:C6     | 2.42                     | 0.55              |
| 1:CA:806:C:H2'    | 1:CA:807:A:H8     | 1.71                     | 0.55              |
| 1:CA:1526:G:H5''  | 21:CU:38:GLU:HG2  | 1.89                     | 0.55              |
| 3:CD:44:LYS:O     | 3:CD:44:LYS:HD3   | 2.07                     | 0.55              |
| 10:CK:19:VAL:CG2  | 10:CK:34:THR:HG22 | 2.31                     | 0.55              |
| 11:CL:73:LEU:HD21 | 11:CL:103:CYS:HA  | 1.89                     | 0.55              |
| 22:DA:51:G:O2'    | 22:DA:52:A:H5''   | 2.06                     | 0.55              |
| 23:DB:639:U:H2'   | 23:DB:640:C:H6    | 1.69                     | 0.55              |
| 23:DB:947:A:O2'   | 23:DB:984:A:H2    | 1.90                     | 0.55              |
| 23:DB:1061:U:H4'  | 23:DB:1070:A:O3'  | 2.07                     | 0.55              |
| 23:DB:1803:A:H5'  | 25:DC:255:LYS:HD3 | 1.88                     | 0.55              |
| 23:DB:2262:U:OP1  | 23:DB:2387:U:O2'  | 2.23                     | 0.55              |
| 23:DB:2756:U:H4'  | 23:DB:2757:A:OP1  | 2.06                     | 0.55              |
| 23:DB:2825:G:H2'  | 23:DB:2826:A:H5'  | 1.89                     | 0.55              |
| 25:DC:19:VAL:HG12 | 25:DC:20:ASN:H    | 1.70                     | 0.55              |
| 26:DD:5:VAL:HG12  | 26:DD:6:GLY:N     | 2.21                     | 0.55              |
| 26:DD:138:LEU:CD1 | 26:DD:142:VAL:HB  | 2.37                     | 0.55              |
| 35:DN:110:MET:O   | 35:DN:111:ALA:HB3 | 2.07                     | 0.55              |
| 39:DR:66:HIS:HA   | 39:DR:98:ILE:HA   | 1.89                     | 0.55              |
| 42:DU:11:ILE:HB   | 42:DU:69:VAL:CG2  | 2.35                     | 0.55              |
| 42:DU:27:VAL:HG12 | 42:DU:33:VAL:HG13 | 1.87                     | 0.55              |
| 43:DW:18:LYS:HZ2  | 43:DW:18:LYS:HB2  | 1.69                     | 0.55              |
| 46:DZ:64:PHE:C    | 46:DZ:67:PRO:HD2  | 2.31                     | 0.55              |
| 51:D4:26:ILE:HD11 | 51:D4:34:LYS:HA   | 1.88                     | 0.55              |
| 1:AA:913:A:H1'    | 1:AA:914:A:O4'    | 2.06                     | 0.55              |
| 2:AC:166:TRP:HA   | 2:AC:166:TRP:CE3  | 2.41                     | 0.55              |
| 16:AQ:63:CYS:SG   | 16:AQ:73:THR:HG23 | 2.47                     | 0.55              |
| 18:AS:49:ALA:HB1  | 18:AS:56:HIS:CB   | 2.31                     | 0.55              |
| 23:BB:142:A:O2'   | 23:BB:143:C:H5'   | 2.07                     | 0.55              |
| 23:BB:395:U:H2'   | 23:BB:396:G:N7    | 2.21                     | 0.55              |
| 23:BB:566:U:O2'   | 23:BB:567:U:H5'   | 2.06                     | 0.55              |
| 23:BB:1551:A:H3'  | 23:BB:1552:A:H5'' | 1.87                     | 0.55              |
| 23:BB:1754:A:OP2  | 37:BP:94:ALA:HB1  | 2.06                     | 0.55              |
| 23:BB:2047:C:H2'  | 23:BB:2048:G:C8   | 2.42                     | 0.55              |
| 23:BB:2393:U:H5'  | 33:BL:62:PRO:CD   | 2.36                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:2471:A:O2'   | 23:BB:2472:G:C8    | 2.54                     | 0.55              |
| 23:BB:2557:G:H2'   | 23:BB:2558:C:H6    | 1.71                     | 0.55              |
| 26:BD:31:ALA:HA    | 26:BD:51:THR:OG1   | 2.07                     | 0.55              |
| 26:BD:93:GLY:O     | 26:BD:94:GLN:HG3   | 2.06                     | 0.55              |
| 29:BG:89:VAL:HG12  | 29:BG:159:LYS:HA   | 1.89                     | 0.55              |
| 31:BJ:112:GLY:O    | 31:BJ:116:ARG:HB2  | 2.06                     | 0.55              |
| 34:BM:7:THR:HG22   | 34:BM:8:LYS:N      | 2.17                     | 0.55              |
| 36:BO:56:LYS:HE3   | 36:BO:57:ALA:N     | 2.22                     | 0.55              |
| 40:BS:70:LYS:HD2   | 40:BS:110:ARG:HG3  | 1.88                     | 0.55              |
| 42:BU:5:ARG:HG2    | 42:BU:6:ARG:N      | 2.20                     | 0.55              |
| 43:BW:45:HIS:HB2   | 43:BW:67:LYS:CE    | 2.37                     | 0.55              |
| 1:CA:129:A:H1'     | 1:CA:130:A:C8      | 2.41                     | 0.55              |
| 1:CA:219:U:H2'     | 1:CA:220:G:C8      | 2.42                     | 0.55              |
| 1:CA:389:A:N3      | 1:CA:389:A:H2'     | 2.22                     | 0.55              |
| 1:CA:412:A:N1      | 3:CD:30:LYS:HG3    | 2.20                     | 0.55              |
| 1:CA:462:G:H3'     | 1:CA:463:U:H5''    | 1.88                     | 0.55              |
| 1:CA:824:G:H2'     | 1:CA:825:A:H8      | 1.71                     | 0.55              |
| 1:CA:1221:G:O3'    | 18:CS:76:THR:HG21  | 2.06                     | 0.55              |
| 1:CA:1226:C:O2'    | 1:CA:1227:A:H5'    | 2.07                     | 0.55              |
| 1:CA:1335:U:H5''   | 1:CA:1337:G:N2     | 2.21                     | 0.55              |
| 3:CD:117:VAL:HG12  | 3:CD:130:ASN:CA    | 2.37                     | 0.55              |
| 5:CF:81:ASN:O      | 5:CF:84:VAL:HG12   | 2.06                     | 0.55              |
| 8:CI:30:ASN:C      | 8:CI:32:ARG:H      | 2.14                     | 0.55              |
| 8:CI:49:GLN:N      | 8:CI:50:PRO:HD2    | 2.22                     | 0.55              |
| 12:CM:44:ILE:HA    | 12:CM:47:LEU:HD21  | 1.89                     | 0.55              |
| 16:CQ:6:THR:HG23   | 16:CQ:59:GLU:OE1   | 2.06                     | 0.55              |
| 18:CS:11:ASP:HB3   | 18:CS:13:HIS:CE1   | 2.42                     | 0.55              |
| 23:DB:705:A:N6     | 23:DB:726:G:O2'    | 2.39                     | 0.55              |
| 23:DB:1099:G:P     | 52:DI:4:VAL:N      | 2.65                     | 0.55              |
| 23:DB:1219:U:H2'   | 23:DB:1220:G:C8    | 2.41                     | 0.55              |
| 23:DB:1405:U:H2'   | 23:DB:1406:U:H6    | 1.72                     | 0.55              |
| 23:DB:1824:G:O2'   | 25:DC:244:VAL:HG21 | 2.06                     | 0.55              |
| 23:DB:2078:C:O2'   | 23:DB:2079:U:H5'   | 2.06                     | 0.55              |
| 23:DB:2080:A:H5'   | 46:DZ:17:SER:CB    | 2.37                     | 0.55              |
| 23:DB:2230:G:H2'   | 23:DB:2231:U:C6    | 2.42                     | 0.55              |
| 23:DB:2527:C:O4'   | 51:D4:1:MET:HE2    | 2.06                     | 0.55              |
| 23:DB:2642:G:OP1   | 31:DJ:84:ILE:HG21  | 2.06                     | 0.55              |
| 24:DV:8:VAL:HG12   | 24:DV:38:LEU:HD11  | 1.89                     | 0.55              |
| 27:DE:149:ILE:HD11 | 27:DE:187:VAL:H    | 1.72                     | 0.55              |
| 29:DG:10:VAL:HG12  | 29:DG:10:VAL:O     | 2.05                     | 0.55              |
| 31:DJ:44:TYR:HE2   | 31:DJ:50:THR:HB    | 1.71                     | 0.55              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:DJ:135:GLN:NE2 | 31:DJ:137:PRO:HB2  | 2.19                     | 0.55              |
| 33:DL:108:ALA:HB3 | 33:DL:125:LEU:CB   | 2.37                     | 0.55              |
| 34:DM:71:LYS:O    | 34:DM:73:ILE:HG12  | 2.07                     | 0.55              |
| 34:DM:133:LYS:HD2 | 34:DM:134:THR:H    | 1.71                     | 0.55              |
| 38:DQ:23:TYR:HB2  | 38:DQ:28:SER:HB3   | 1.89                     | 0.55              |
| 40:DS:34:ASP:HA   | 40:DS:37:THR:HG22  | 1.88                     | 0.55              |
| 42:DU:94:PHE:CD2  | 42:DU:100:GLU:HG2  | 2.42                     | 0.55              |
| 44:DX:23:ARG:HA   | 44:DX:26:PHE:CD1   | 2.42                     | 0.55              |
| 47:D0:41:HIS:CG   | 47:D0:42:ILE:N     | 2.70                     | 0.55              |
| 50:D3:2:LYS:HB2   | 50:D3:2:LYS:HZ2    | 1.72                     | 0.55              |
| 1:AA:70:U:H1'     | 1:AA:71:A:N7       | 2.22                     | 0.55              |
| 1:AA:173:U:H5'    | 1:AA:197:A:O4'     | 2.07                     | 0.55              |
| 1:AA:220:G:O2'    | 1:AA:221:C:H5'     | 2.06                     | 0.55              |
| 1:AA:736:C:H4'    | 5:AF:88:MET:HE3    | 1.87                     | 0.55              |
| 1:AA:801:U:H2'    | 1:AA:802:A:C8      | 2.42                     | 0.55              |
| 1:AA:806:C:H2'    | 1:AA:807:A:H8      | 1.72                     | 0.55              |
| 1:AA:1289:A:C2'   | 1:AA:1290:G:H5'    | 2.35                     | 0.55              |
| 3:AD:152:SER:O    | 3:AD:155:LYS:HG3   | 2.07                     | 0.55              |
| 4:AE:80:LEU:HB2   | 4:AE:97:PRO:HB3    | 1.87                     | 0.55              |
| 5:AF:9:MET:HE1    | 17:AR:64:LEU:HA    | 1.89                     | 0.55              |
| 6:AG:71:THR:O     | 6:AG:72:VAL:HG13   | 2.06                     | 0.55              |
| 8:AI:56:MET:SD    | 8:AI:57:VAL:N      | 2.80                     | 0.55              |
| 16:AQ:58:VAL:HB   | 16:AQ:74:LEU:HD23  | 1.88                     | 0.55              |
| 22:BA:6:G:H2'     | 22:BA:7:G:H8       | 1.69                     | 0.55              |
| 23:BB:36:G:N2     | 23:BB:37:C:H1'     | 2.22                     | 0.55              |
| 23:BB:458:G:P     | 49:B2:39:ARG:HH22  | 2.29                     | 0.55              |
| 23:BB:589:U:H2'   | 23:BB:590:A:H8     | 1.72                     | 0.55              |
| 23:BB:921:C:O2'   | 23:BB:922:C:H5'    | 2.06                     | 0.55              |
| 23:BB:1515:A:H5'  | 23:BB:1557:C:H5'   | 1.88                     | 0.55              |
| 23:BB:2138:G:H2'  | 23:BB:2139:U:C6    | 2.42                     | 0.55              |
| 24:BV:77:VAL:HG12 | 34:BM:133:LYS:NZ   | 2.21                     | 0.55              |
| 29:BG:77:GLY:HA3  | 29:BG:135:ALA:O    | 2.07                     | 0.55              |
| 30:BH:75:LEU:HD23 | 30:BH:76:GLU:H     | 1.71                     | 0.55              |
| 32:BK:97:THR:OG1  | 32:BK:98:ARG:HD2   | 2.06                     | 0.55              |
| 36:BO:76:LYS:HB2  | 36:BO:106:LEU:HD22 | 1.88                     | 0.55              |
| 37:BP:109:ILE:O   | 37:BP:110:LYS:C    | 2.50                     | 0.55              |
| 47:B0:6:LYS:HA    | 47:B0:6:LYS:HZ2    | 1.70                     | 0.55              |
| 1:CA:230:G:O2'    | 1:CA:231:U:H5'     | 2.07                     | 0.55              |
| 1:CA:1157:A:H5'   | 1:CA:1158:C:C6     | 2.42                     | 0.55              |
| 6:CG:106:ALA:HB1  | 6:CG:132:THR:OG1   | 2.07                     | 0.55              |
| 8:CI:50:PRO:O     | 8:CI:54:VAL:HG22   | 2.06                     | 0.55              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:CK:17:ASP:OD1  | 10:CK:36:ARG:HG3  | 2.06                     | 0.55              |
| 11:CL:54:VAL:CG1  | 11:CL:79:ILE:HD11 | 2.37                     | 0.55              |
| 18:CS:30:LEU:HD12 | 18:CS:48:ILE:HG12 | 1.88                     | 0.55              |
| 23:DB:90:U:OP2    | 23:DB:91:A:H3'    | 2.07                     | 0.55              |
| 23:DB:278:A:H2'   | 23:DB:278:A:N3    | 2.20                     | 0.55              |
| 23:DB:321:U:OP2   | 27:DE:130:LYS:HA  | 2.07                     | 0.55              |
| 23:DB:667:U:H2'   | 23:DB:668:A:O4'   | 2.07                     | 0.55              |
| 23:DB:845:A:C6    | 23:DB:847:U:H1'   | 2.42                     | 0.55              |
| 23:DB:1444:G:H2'  | 23:DB:1445:G:C8   | 2.40                     | 0.55              |
| 23:DB:1651:G:H4'  | 35:DN:39:PRO:HG2  | 1.89                     | 0.55              |
| 23:DB:2213:U:O2   | 23:DB:2213:U:H2'  | 2.07                     | 0.55              |
| 23:DB:2282:G:O2'  | 23:DB:2283:C:P    | 2.64                     | 0.55              |
| 25:DC:216:ARG:HB3 | 25:DC:217:PRO:CD  | 2.37                     | 0.55              |
| 26:DD:118:PHE:HA  | 26:DD:164:GLN:HA  | 1.89                     | 0.55              |
| 28:DF:98:PHE:HA   | 28:DF:101:ARG:NE  | 2.18                     | 0.55              |
| 35:DN:4:ARG:H     | 35:DN:4:ARG:NH2   | 2.05                     | 0.55              |
| 37:DP:52:ARG:HD2  | 37:DP:60:VAL:HG13 | 1.88                     | 0.55              |
| 40:DS:72:THR:HB   | 40:DS:109:ASP:HB2 | 1.88                     | 0.55              |
| 47:D0:41:HIS:NE2  | 47:D0:42:ILE:HG22 | 2.22                     | 0.55              |
| 47:D0:42:ILE:O    | 47:D0:46:GLY:N    | 2.39                     | 0.55              |
| 1:AA:219:U:H2'    | 1:AA:220:G:C8     | 2.42                     | 0.55              |
| 1:AA:279:A:H4'    | 1:AA:280:C:OP2    | 2.06                     | 0.55              |
| 1:AA:389:A:H2'    | 1:AA:389:A:N3     | 2.22                     | 0.55              |
| 1:AA:426:U:H2'    | 1:AA:427:U:C6     | 2.41                     | 0.55              |
| 1:AA:521:G:OP2    | 11:AL:50:LYS:HE3  | 2.07                     | 0.55              |
| 3:AD:24:VAL:C     | 3:AD:25:ARG:HD2   | 2.31                     | 0.55              |
| 3:AD:115:GLN:HG3  | 3:AD:119:HIS:CE1  | 2.41                     | 0.55              |
| 10:AK:15:VAL:HG11 | 10:AK:35:ASP:HB2  | 1.88                     | 0.55              |
| 14:AO:78:THR:HA   | 14:AO:81:ILE:HG12 | 1.89                     | 0.55              |
| 16:AQ:18:LYS:HA   | 16:AQ:47:ASP:O    | 2.07                     | 0.55              |
| 17:AR:21:ASP:OD2  | 17:AR:23:LYS:HG3  | 2.06                     | 0.55              |
| 20:AB:30:ILE:HA   | 20:AB:39:ILE:O    | 2.07                     | 0.55              |
| 23:BB:280:U:H2'   | 23:BB:281:C:C6    | 2.42                     | 0.55              |
| 23:BB:329:G:O6    | 42:BU:16:LYS:HE2  | 2.07                     | 0.55              |
| 23:BB:856:G:H21   | 43:BW:22:VAL:HG11 | 1.72                     | 0.55              |
| 23:BB:1405:U:H2'  | 23:BB:1406:U:H6   | 1.71                     | 0.55              |
| 23:BB:1591:A:H2'  | 23:BB:1592:C:C6   | 2.42                     | 0.55              |
| 23:BB:1904:G:O2'  | 23:BB:1905:C:H5'  | 2.06                     | 0.55              |
| 23:BB:2236:U:H2'  | 23:BB:2237:G:O4'  | 2.07                     | 0.55              |
| 23:BB:2265:U:H3'  | 23:BB:2266:A:C5'  | 2.36                     | 0.55              |
| 23:BB:2307:G:H4'  | 23:BB:2311:A:N6   | 2.22                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:2335:A:OP2  | 36:BO:9:ARG:HG3    | 2.07                     | 0.55              |
| 23:BB:2839:G:H2'  | 23:BB:2840:C:C6    | 2.41                     | 0.55              |
| 25:BC:42:ARG:CG   | 25:BC:43:ASN:N     | 2.62                     | 0.55              |
| 26:BD:48:ILE:HG13 | 26:BD:80:TRP:CD1   | 2.41                     | 0.55              |
| 26:BD:149:ASN:C   | 26:BD:150:GLN:HG2  | 2.32                     | 0.55              |
| 32:BK:87:LEU:HA   | 32:BK:95:ILE:H     | 1.72                     | 0.55              |
| 33:BL:63:LYS:HB2  | 50:B3:11:LYS:HG3   | 1.87                     | 0.55              |
| 33:BL:77:ILE:CB   | 33:BL:110:VAL:HG22 | 2.31                     | 0.55              |
| 34:BM:42:THR:O    | 34:BM:44:ARG:N     | 2.39                     | 0.55              |
| 39:BR:22:LEU:O    | 39:BR:96:VAL:HG22  | 2.06                     | 0.55              |
| 48:B1:31:GLU:CG   | 48:B1:32:LYS:H     | 2.19                     | 0.55              |
| 49:B2:43:THR:O    | 49:B2:44:VAL:C     | 2.49                     | 0.55              |
| 52:BI:49:GLU:CG   | 52:BI:54:ILE:HD11  | 2.37                     | 0.55              |
| 1:CA:16:A:N1      | 1:CA:919:A:H2      | 2.04                     | 0.55              |
| 1:CA:254:G:O2'    | 1:CA:255:G:H5'     | 2.07                     | 0.55              |
| 1:CA:1062:U:H2'   | 1:CA:1063:C:C6     | 2.42                     | 0.55              |
| 1:CA:1248:A:H2    | 8:CI:71:ILE:HD11   | 1.70                     | 0.55              |
| 1:CA:1386:G:H2'   | 1:CA:1387:G:C8     | 2.42                     | 0.55              |
| 3:CD:78:ALA:HB1   | 3:CD:85:THR:HA     | 1.88                     | 0.55              |
| 11:CL:120:ARG:HD3 | 11:CL:121:PRO:HD2  | 1.88                     | 0.55              |
| 13:CN:68:ARG:NH2  | 13:CN:80:ARG:HH12  | 2.05                     | 0.55              |
| 20:CB:205:ALA:HB3 | 20:CB:208:ALA:HB3  | 1.88                     | 0.55              |
| 23:DB:741:U:H2'   | 23:DB:742:A:C8     | 2.41                     | 0.55              |
| 23:DB:1432:G:O2'  | 23:DB:1433:A:H5'   | 2.07                     | 0.55              |
| 23:DB:1564:C:O2'  | 23:DB:1565:C:H5'   | 2.06                     | 0.55              |
| 23:DB:2216:G:H2'  | 23:DB:2217:G:H8    | 1.72                     | 0.55              |
| 23:DB:2895:G:H2'  | 23:DB:2896:C:H6    | 1.66                     | 0.55              |
| 29:DG:79:THR:HG23 | 29:DG:80:GLU:N     | 2.22                     | 0.55              |
| 32:DK:108:ARG:NH2 | 37:DP:36:LYS:H     | 2.04                     | 0.55              |
| 37:DP:59:THR:HA   | 37:DP:76:HIS:HA    | 1.89                     | 0.55              |
| 37:DP:93:LYS:CG   | 37:DP:96:LEU:HA    | 2.26                     | 0.55              |
| 39:DR:4:VAL:HA    | 39:DR:43:ASN:CG    | 2.32                     | 0.55              |
| 39:DR:41:ILE:O    | 39:DR:43:ASN:N     | 2.39                     | 0.55              |
| 43:DW:20:LEU:HD11 | 43:DW:31:LEU:HD12  | 1.88                     | 0.55              |
| 46:DZ:3:LYS:H     | 46:DZ:3:LYS:HD2    | 1.72                     | 0.55              |
| 1:AA:415:A:H3'    | 1:AA:416:G:H8      | 1.72                     | 0.55              |
| 1:AA:1307:U:H2'   | 1:AA:1308:U:C6     | 2.42                     | 0.55              |
| 3:AD:98:ASP:HB2   | 3:AD:132:ALA:HB1   | 1.88                     | 0.55              |
| 6:AG:99:ALA:O     | 6:AG:103:ILE:HG13  | 2.07                     | 0.55              |
| 8:AI:64:ILE:HD13  | 8:AI:78:ILE:CG2    | 2.37                     | 0.55              |
| 13:AN:30:ILE:C    | 13:AN:32:ASP:H     | 2.14                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:AB:53:LEU:HD11  | 20:AB:216:VAL:HA   | 1.87                     | 0.55              |
| 23:BB:62:U:H3'     | 23:BB:63:A:H8      | 1.72                     | 0.55              |
| 23:BB:64:A:H2'     | 23:BB:65:U:C6      | 2.42                     | 0.55              |
| 23:BB:235:U:H2'    | 23:BB:236:C:C6     | 2.42                     | 0.55              |
| 23:BB:866:A:H61    | 23:BB:913:U:C4'    | 2.19                     | 0.55              |
| 23:BB:1327:A:H2'   | 23:BB:1328:A:O4'   | 2.06                     | 0.55              |
| 23:BB:1843:C:H5''  | 25:BC:252:LYS:HZ3  | 1.72                     | 0.55              |
| 23:BB:2093:G:O2'   | 23:BB:2094:A:H5'   | 2.07                     | 0.55              |
| 25:BC:260:LYS:HB2  | 25:BC:261:ARG:HE   | 1.71                     | 0.55              |
| 28:BF:165:GLY:HA2  | 28:BF:168:LEU:HD21 | 1.88                     | 0.55              |
| 30:BH:11:ASN:ND2   | 30:BH:12:LEU:N     | 2.55                     | 0.55              |
| 37:BP:1:SER:HA     | 37:BP:4:ILE:HD12   | 1.88                     | 0.55              |
| 37:BP:23:ASP:N     | 37:BP:93:LYS:HE2   | 2.22                     | 0.55              |
| 37:BP:112:ARG:CA   | 37:BP:112:ARG:HH11 | 2.20                     | 0.55              |
| 42:BU:11:ILE:HG23  | 42:BU:20:LYS:O     | 2.07                     | 0.55              |
| 43:BW:21:GLY:HA3   | 43:BW:32:ALA:CB    | 2.36                     | 0.55              |
| 1:CA:118:U:O4      | 1:CA:288:A:H2'     | 2.07                     | 0.55              |
| 1:CA:454:G:O2'     | 1:CA:455:G:H5'     | 2.07                     | 0.55              |
| 1:CA:985:C:H2'     | 1:CA:986:U:H6      | 1.71                     | 0.55              |
| 1:CA:1068:G:N7     | 1:CA:1094:G:H2'    | 2.22                     | 0.55              |
| 3:CD:118:SER:HA    | 3:CD:130:ASN:HB2   | 1.87                     | 0.55              |
| 9:CJ:40:ILE:HG13   | 9:CJ:73:LEU:HB3    | 1.89                     | 0.55              |
| 16:CQ:68:LYS:O     | 16:CQ:70:LYS:N     | 2.40                     | 0.55              |
| 16:CQ:74:LEU:HD22  | 16:CQ:75:VAL:N     | 2.22                     | 0.55              |
| 22:DA:76:G:H2'     | 22:DA:77:U:C6      | 2.38                     | 0.55              |
| 22:DA:103:U:O2'    | 22:DA:104:A:H5'    | 2.07                     | 0.55              |
| 23:DB:1351:C:O2'   | 23:DB:1571:A:H1'   | 2.06                     | 0.55              |
| 23:DB:1921:G:O2'   | 23:DB:1922:G:H5'   | 2.07                     | 0.55              |
| 23:DB:2239:G:OP1   | 25:DC:246:PRO:HG3  | 2.07                     | 0.55              |
| 23:DB:2400:G:O2'   | 23:DB:2401:U:H5'   | 2.07                     | 0.55              |
| 23:DB:2848:G:H1'   | 23:DB:2868:A:H61   | 1.72                     | 0.55              |
| 24:DV:26:PHE:HE2   | 24:DV:44:HIS:HA    | 1.72                     | 0.55              |
| 27:DE:112:LEU:HD12 | 27:DE:115:GLN:NE2  | 2.22                     | 0.55              |
| 29:DG:34:ARG:NH1   | 29:DG:70:LEU:HG    | 2.22                     | 0.55              |
| 30:DH:4:ILE:HD13   | 30:DH:4:ILE:H      | 1.71                     | 0.55              |
| 31:DJ:44:TYR:CD1   | 31:DJ:45:THR:N     | 2.71                     | 0.55              |
| 33:DL:33:ARG:CG    | 39:DR:85:LYS:HZ3   | 2.20                     | 0.55              |
| 38:DQ:52:ARG:HD3   | 38:DQ:53:LYS:HZ1   | 1.72                     | 0.55              |
| 39:DR:86:GLN:HG3   | 39:DR:87:GLN:HG2   | 1.89                     | 0.55              |
| 40:DS:58:ALA:O     | 40:DS:62:ASP:HB3   | 2.06                     | 0.55              |
| 40:DS:85:ILE:HD13  | 40:DS:86:MET:N     | 2.21                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:DT:48:GLN:HG3   | 41:DT:49:LYS:N     | 2.21                     | 0.55              |
| 41:DT:53:VAL:HA    | 41:DT:93:LEU:HG    | 1.88                     | 0.55              |
| 42:DU:27:VAL:HG12  | 42:DU:33:VAL:HG22  | 1.87                     | 0.55              |
| 42:DU:96:LYS:HD3   | 42:DU:97:SER:N     | 2.21                     | 0.55              |
| 43:DW:47:GLY:CA    | 43:DW:71:LYS:HB3   | 2.34                     | 0.55              |
| 1:AA:132:C:H5''    | 19:AT:68:LYS:CE    | 2.37                     | 0.55              |
| 1:AA:921:U:H2'     | 1:AA:922:G:O4'     | 2.07                     | 0.55              |
| 1:AA:1033:G:H2'    | 1:AA:1034:G:O4'    | 2.07                     | 0.55              |
| 1:AA:1494:G:O2'    | 1:AA:1495:U:H5'    | 2.06                     | 0.55              |
| 7:AH:31:LEU:O      | 7:AH:35:ILE:HG13   | 2.07                     | 0.55              |
| 15:AP:18:GLN:NE2   | 15:AP:35:ARG:HD2   | 2.22                     | 0.55              |
| 16:AQ:20:ILE:HG21  | 16:AQ:52:CYS:SG    | 2.47                     | 0.55              |
| 21:AU:26:GLY:C     | 21:AU:28:LEU:H     | 2.15                     | 0.55              |
| 22:BA:91:C:O2'     | 22:BA:92:C:H5'     | 2.07                     | 0.55              |
| 23:BB:38:A:C8      | 27:BE:46:GLN:CD    | 2.85                     | 0.55              |
| 23:BB:607:U:O4     | 23:BB:620:G:H5''   | 2.07                     | 0.55              |
| 23:BB:994:C:H3'    | 38:BQ:53:LYS:HE2   | 1.88                     | 0.55              |
| 23:BB:1001:A:H2'   | 23:BB:1002:G:O4'   | 2.07                     | 0.55              |
| 23:BB:1300:G:H5'   | 23:BB:1301:A:N3    | 2.22                     | 0.55              |
| 23:BB:1439:A:C6    | 23:BB:1552:A:C5    | 2.95                     | 0.55              |
| 23:BB:2104:C:H2'   | 23:BB:2105:U:H5    | 1.72                     | 0.55              |
| 25:BC:68:ARG:HH22  | 25:BC:190:THR:HG23 | 1.72                     | 0.55              |
| 25:BC:80:LEU:HA    | 25:BC:91:ALA:HA    | 1.89                     | 0.55              |
| 26:BD:35:THR:CG2   | 26:BD:46:ARG:HH22  | 2.20                     | 0.55              |
| 27:BE:35:TYR:C     | 27:BE:37:ALA:H     | 2.15                     | 0.55              |
| 28:BF:35:LEU:HD22  | 28:BF:56:LEU:HD21  | 1.88                     | 0.55              |
| 30:BH:121:VAL:HG21 | 30:BH:128:HIS:HE2  | 1.72                     | 0.55              |
| 33:BL:39:LYS:CB    | 33:BL:46:VAL:HG13  | 2.37                     | 0.55              |
| 33:BL:71:ALA:O     | 33:BL:72:ALA:C     | 2.50                     | 0.55              |
| 33:BL:77:ILE:HD12  | 33:BL:110:VAL:CG2  | 2.37                     | 0.55              |
| 33:BL:77:ILE:CD1   | 33:BL:92:LEU:HD13  | 2.32                     | 0.55              |
| 36:BO:12:THR:OG1   | 36:BO:13:ARG:HD2   | 2.07                     | 0.55              |
| 42:BU:24:VAL:C     | 42:BU:25:LYS:HD3   | 2.32                     | 0.55              |
| 44:BX:38:GLN:O     | 44:BX:39:GLN:HG3   | 2.07                     | 0.55              |
| 45:BY:6:ILE:HD13   | 45:BY:6:ILE:N      | 2.22                     | 0.55              |
| 48:B1:10:LEU:HD13  | 48:B1:25:ASN:HD22  | 1.71                     | 0.55              |
| 1:CA:500:G:H5''    | 11:CL:120:ARG:HH21 | 1.71                     | 0.55              |
| 1:CA:610:U:O2      | 1:CA:610:U:O4'     | 2.25                     | 0.55              |
| 1:CA:1297:G:H4'    | 1:CA:1298:U:H5'    | 1.88                     | 0.55              |
| 1:CA:1355:G:H2'    | 1:CA:1356:G:C8     | 2.41                     | 0.55              |
| 2:CC:58:ARG:HA     | 2:CC:63:ILE:HA     | 1.88                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:CD:16:THR:HG22   | 3:CD:17:ASP:H      | 1.71                     | 0.55              |
| 3:CD:123:MET:HE3   | 3:CD:126:GLY:O     | 2.06                     | 0.55              |
| 6:CG:91:ARG:O      | 6:CG:95:ARG:HG3    | 2.07                     | 0.55              |
| 10:CK:106:ILE:HD11 | 10:CK:109:ILE:HG13 | 1.87                     | 0.55              |
| 12:CM:80:MET:HA    | 12:CM:87:GLY:CA    | 2.37                     | 0.55              |
| 13:CN:82:LYS:O     | 13:CN:85:GLU:HB2   | 2.07                     | 0.55              |
| 19:CT:66:ILE:HG23  | 19:CT:70:LYS:HG3   | 1.87                     | 0.55              |
| 20:CB:101:THR:HG22 | 20:CB:174:GLU:OE1  | 2.06                     | 0.55              |
| 22:DA:66:A:O2'     | 22:DA:67:G:H8      | 1.90                     | 0.55              |
| 23:DB:106:C:H2'    | 23:DB:107:G:H8     | 1.71                     | 0.55              |
| 23:DB:1300:G:H5'   | 23:DB:1301:A:N3    | 2.22                     | 0.55              |
| 23:DB:1934:C:O2'   | 23:DB:1935:G:H5'   | 2.07                     | 0.55              |
| 23:DB:2228:G:H2'   | 23:DB:2229:U:C6    | 2.42                     | 0.55              |
| 23:DB:2553:G:H2'   | 23:DB:2554:U:H4'   | 1.89                     | 0.55              |
| 23:DB:2729:G:H2'   | 23:DB:2730:C:H6    | 1.72                     | 0.55              |
| 23:DB:2843:G:O2'   | 23:DB:2844:G:H5'   | 2.07                     | 0.55              |
| 24:DV:24:ASN:HB3   | 24:DV:45:ASP:OD1   | 2.06                     | 0.55              |
| 24:DV:65:VAL:C     | 24:DV:67:GLY:H     | 2.15                     | 0.55              |
| 25:DC:21:PRO:C     | 25:DC:202:ARG:HD2  | 2.32                     | 0.55              |
| 29:DG:126:THR:HG23 | 29:DG:129:GLU:H    | 1.72                     | 0.55              |
| 30:DH:5:LEU:HD13   | 30:DH:35:LYS:CE    | 2.37                     | 0.55              |
| 31:DJ:41:LYS:NZ    | 31:DJ:45:THR:HA    | 2.22                     | 0.55              |
| 32:DK:64:ARG:HD3   | 32:DK:83:ALA:HB2   | 1.89                     | 0.55              |
| 33:DL:109:LYS:O    | 33:DL:110:VAL:HG13 | 2.07                     | 0.55              |
| 37:DP:55:HIS:C     | 37:DP:57:ALA:N     | 2.64                     | 0.55              |
| 40:DS:86:MET:HG3   | 40:DS:87:PRO:HD2   | 1.89                     | 0.55              |
| 41:DT:31:VAL:HG13  | 41:DT:32:LEU:N     | 2.16                     | 0.55              |
| 52:DI:102:ARG:HG3  | 52:DI:141:ASP:HB2  | 1.89                     | 0.55              |
| 1:AA:118:U:O4      | 1:AA:288:A:H2'     | 2.07                     | 0.54              |
| 1:AA:1110:A:H2'    | 1:AA:1111:A:H5'    | 1.89                     | 0.54              |
| 2:AC:180:ASP:C     | 2:AC:181:ILE:HD12  | 2.31                     | 0.54              |
| 3:AD:111:ALA:O     | 3:AD:114:ARG:HB3   | 2.07                     | 0.54              |
| 12:AM:3:ILE:HG23   | 12:AM:56:ARG:HG2   | 1.87                     | 0.54              |
| 13:AN:33:VAL:HG23  | 13:AN:40:ARG:NH2   | 2.23                     | 0.54              |
| 20:AB:206:ILE:HD13 | 20:AB:206:ILE:C    | 2.32                     | 0.54              |
| 23:BB:26:G:H1'     | 23:BB:514:A:H61    | 1.70                     | 0.54              |
| 23:BB:372:G:N2     | 23:BB:401:A:OP2    | 2.35                     | 0.54              |
| 23:BB:528:A:C2     | 23:BB:2043:C:H4'   | 2.42                     | 0.54              |
| 23:BB:593:U:H2'    | 23:BB:594:U:C6     | 2.41                     | 0.54              |
| 23:BB:729:G:H4'    | 23:BB:763:G:H5'    | 1.88                     | 0.54              |
| 23:BB:764:A:H5''   | 25:BC:208:GLY:CA   | 2.37                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:1166:G:H2'   | 23:BB:1167:C:C6    | 2.43                     | 0.54              |
| 23:BB:1565:C:OP1   | 25:BC:23:LEU:HD23  | 2.08                     | 0.54              |
| 23:BB:1637:A:H2'   | 23:BB:1638:C:H6    | 1.73                     | 0.54              |
| 23:BB:1774:C:O2    | 23:BB:1774:C:C2'   | 2.54                     | 0.54              |
| 23:BB:1821:A:H5'   | 25:BC:155:ARG:HD2  | 1.89                     | 0.54              |
| 23:BB:1921:G:O2'   | 23:BB:1922:G:H5'   | 2.07                     | 0.54              |
| 23:BB:2320:U:H3'   | 23:BB:2321:U:H5'   | 1.88                     | 0.54              |
| 23:BB:2575:C:H5''  | 26:BD:149:ASN:N    | 2.22                     | 0.54              |
| 26:BD:167:ASN:HD22 | 26:BD:167:ASN:N    | 2.04                     | 0.54              |
| 27:BE:49:ARG:HB2   | 27:BE:49:ARG:NH1   | 2.23                     | 0.54              |
| 28:BF:37:MET:HG2   | 28:BF:86:CYS:HB2   | 1.89                     | 0.54              |
| 30:BH:69:ALA:HB2   | 30:BH:139:PHE:O    | 2.07                     | 0.54              |
| 31:BJ:37:ARG:NH2   | 31:BJ:110:PRO:HG3  | 2.22                     | 0.54              |
| 33:BL:79:LEU:CA    | 33:BL:113:ALA:HB3  | 2.37                     | 0.54              |
| 37:BP:30:TRP:H     | 37:BP:30:TRP:CD1   | 2.23                     | 0.54              |
| 43:BW:4:LYS:HD3    | 43:BW:4:LYS:C      | 2.32                     | 0.54              |
| 44:BX:38:GLN:H     | 44:BX:38:GLN:HE21  | 1.54                     | 0.54              |
| 52:BI:74:PRO:O     | 52:BI:77:VAL:HG22  | 2.07                     | 0.54              |
| 1:CA:598:U:H4'     | 7:CH:85:TYR:CD2    | 2.43                     | 0.54              |
| 1:CA:1077:G:N2     | 1:CA:1080:A:OP2    | 2.40                     | 0.54              |
| 1:CA:1320:C:H41    | 18:CS:36:ARG:HG3   | 1.72                     | 0.54              |
| 4:CE:108:GLY:O     | 4:CE:111:ARG:HB3   | 2.06                     | 0.54              |
| 6:CG:134:VAL:O     | 6:CG:138:GLU:HG3   | 2.06                     | 0.54              |
| 10:CK:13:LYS:HD2   | 10:CK:13:LYS:N     | 2.21                     | 0.54              |
| 14:CO:80:LEU:O     | 14:CO:84:LEU:HD13  | 2.07                     | 0.54              |
| 15:CP:28:ARG:HD3   | 15:CP:29:ASN:OD1   | 2.07                     | 0.54              |
| 16:CQ:83:LEU:N     | 16:CQ:83:LEU:HD22  | 2.22                     | 0.54              |
| 17:CR:54:LEU:O     | 17:CR:58:ILE:HG13  | 2.07                     | 0.54              |
| 21:CU:24:LYS:NZ    | 21:CU:24:LYS:HB3   | 2.22                     | 0.54              |
| 22:DA:49:C:H2'     | 22:DA:50:A:C8      | 2.42                     | 0.54              |
| 23:DB:191:A:O2'    | 23:DB:192:C:H5'    | 2.08                     | 0.54              |
| 23:DB:635:C:H3'    | 33:DL:126:ARG:HH21 | 1.73                     | 0.54              |
| 23:DB:810:U:C2     | 33:DL:37:GLY:HA2   | 2.43                     | 0.54              |
| 23:DB:1022:G:N2    | 23:DB:1142:A:C2    | 2.75                     | 0.54              |
| 23:DB:1291:C:O2'   | 23:DB:1292:G:H5'   | 2.07                     | 0.54              |
| 23:DB:1400:U:H2'   | 23:DB:1401:G:C8    | 2.41                     | 0.54              |
| 23:DB:1773:A:N6    | 25:DC:206:LYS:HE2  | 2.22                     | 0.54              |
| 23:DB:2097:A:H2'   | 23:DB:2098:U:C6    | 2.42                     | 0.54              |
| 23:DB:2646:C:H2'   | 23:DB:2647:U:O4'   | 2.07                     | 0.54              |
| 25:DC:37:SER:H     | 25:DC:62:ARG:HB3   | 1.71                     | 0.54              |
| 27:DE:164:LEU:HD22 | 27:DE:164:LEU:O    | 2.06                     | 0.54              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:DF:134:GLN:O    | 28:DF:135:ILE:C    | 2.48                     | 0.54              |
| 28:DF:140:ILE:HD12 | 28:DF:140:ILE:N    | 2.17                     | 0.54              |
| 29:DG:123:GLU:HG2  | 29:DG:131:VAL:HG13 | 1.89                     | 0.54              |
| 30:DH:113:SER:HB2  | 30:DH:132:PHE:CZ   | 2.42                     | 0.54              |
| 31:DJ:120:ARG:HB3  | 31:DJ:121:LYS:NZ   | 2.22                     | 0.54              |
| 31:DJ:120:ARG:N    | 31:DJ:121:LYS:HZ2  | 2.05                     | 0.54              |
| 32:DK:43:ILE:H     | 32:DK:43:ILE:CD1   | 2.19                     | 0.54              |
| 33:DL:123:ARG:HA   | 33:DL:142:ILE:HA   | 1.88                     | 0.54              |
| 34:DM:101:VAL:HG12 | 34:DM:102:LEU:N    | 2.21                     | 0.54              |
| 35:DN:4:ARG:CZ     | 35:DN:4:ARG:H      | 2.19                     | 0.54              |
| 37:DP:47:ILE:HD13  | 37:DP:63:ILE:HG12  | 1.89                     | 0.54              |
| 41:DT:34:VAL:HG22  | 41:DT:35:ALA:N     | 2.20                     | 0.54              |
| 41:DT:92:ASN:O     | 41:DT:93:LEU:HD12  | 2.06                     | 0.54              |
| 43:DW:36:ILE:HG21  | 43:DW:68:PHE:CE1   | 2.42                     | 0.54              |
| 43:DW:43:LYS:H     | 43:DW:75:ASN:CG    | 2.15                     | 0.54              |
| 44:DX:25:GLN:CD    | 44:DX:29:ARG:HH21  | 2.14                     | 0.54              |
| 48:D1:5:ARG:HA     | 48:D1:28:THR:OG1   | 2.07                     | 0.54              |
| 50:D3:5:THR:O      | 50:D3:5:THR:HG23   | 2.06                     | 0.54              |
| 51:D4:15:LYS:HZ1   | 51:D4:22:VAL:HG12  | 1.71                     | 0.54              |
| 52:DI:49:GLU:CB    | 52:DI:52:LEU:HD12  | 2.37                     | 0.54              |
| 52:DI:99:LYS:HD3   | 52:DI:99:LYS:H     | 1.71                     | 0.54              |
| 1:AA:98:A:H2'      | 1:AA:99:C:C6       | 2.42                     | 0.54              |
| 1:AA:123:U:OP1     | 1:AA:312:C:H5'     | 2.07                     | 0.54              |
| 1:AA:254:G:O2'     | 1:AA:255:G:H5'     | 2.07                     | 0.54              |
| 1:AA:915:A:H2'     | 1:AA:916:U:H5'     | 1.89                     | 0.54              |
| 1:AA:944:G:H1'     | 1:AA:1339:A:N6     | 2.23                     | 0.54              |
| 5:AF:29:ILE:HD13   | 5:AF:64:VAL:HG11   | 1.88                     | 0.54              |
| 10:AK:109:ILE:CG2  | 21:AU:16:ARG:HD2   | 2.37                     | 0.54              |
| 12:AM:95:PRO:HD3   | 12:AM:108:ARG:HG2  | 1.89                     | 0.54              |
| 15:AP:1:MET:HE1    | 15:AP:64:GLY:O     | 2.07                     | 0.54              |
| 15:AP:52:LEU:HG    | 15:AP:75:ILE:HG12  | 1.89                     | 0.54              |
| 16:AQ:80:LYS:HE3   | 16:AQ:80:LYS:C     | 2.32                     | 0.54              |
| 21:AU:34:ARG:HD2   | 21:AU:34:ARG:C     | 2.31                     | 0.54              |
| 22:BA:76:G:H2'     | 22:BA:77:U:C6      | 2.42                     | 0.54              |
| 23:BB:559:G:H1'    | 38:BQ:55:GLN:HE22  | 1.72                     | 0.54              |
| 23:BB:1028:A:H2'   | 23:BB:1029:A:C8    | 2.42                     | 0.54              |
| 23:BB:1227:G:O2'   | 23:BB:1228:G:H5'   | 2.08                     | 0.54              |
| 23:BB:2292:U:H2'   | 23:BB:2293:G:H8    | 1.73                     | 0.54              |
| 23:BB:2467:C:C1'   | 34:BM:118:LYS:HG2  | 2.37                     | 0.54              |
| 23:BB:2512:C:H2'   | 23:BB:2513:A:O4'   | 2.07                     | 0.54              |
| 23:BB:2646:C:H2'   | 23:BB:2647:U:O4'   | 2.07                     | 0.54              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:BC:70:LYS:HE3  | 25:BC:95:TYR:CD2   | 2.43                     | 0.54              |
| 27:BE:143:LEU:CG  | 27:BE:185:LYS:HD2  | 2.33                     | 0.54              |
| 28:BF:7:TYR:HA    | 28:BF:11:VAL:HB    | 1.90                     | 0.54              |
| 28:BF:52:ALA:HA   | 28:BF:148:VAL:HG13 | 1.90                     | 0.54              |
| 29:BG:154:GLU:OE1 | 29:BG:156:TYR:HB2  | 2.07                     | 0.54              |
| 32:BK:98:ARG:HA   | 32:BK:118:LEU:HD22 | 1.89                     | 0.54              |
| 34:BM:40:ARG:HD3  | 34:BM:92:TRP:HB3   | 1.90                     | 0.54              |
| 38:BQ:52:ARG:NH1  | 38:BQ:55:GLN:HE21  | 2.05                     | 0.54              |
| 39:BR:39:LEU:O    | 39:BR:54:VAL:HG12  | 2.06                     | 0.54              |
| 40:BS:44:ALA:O    | 40:BS:47:VAL:HG22  | 2.07                     | 0.54              |
| 42:BU:13:LEU:HG   | 42:BU:69:VAL:HG22  | 1.89                     | 0.54              |
| 42:BU:33:VAL:HG21 | 42:BU:66:VAL:HA    | 1.89                     | 0.54              |
| 1:CA:801:U:H2'    | 1:CA:802:A:C8      | 2.42                     | 0.54              |
| 1:CA:1064:G:H4'   | 1:CA:1065:U:OP1    | 2.06                     | 0.54              |
| 1:CA:1217:C:H2'   | 1:CA:1218:C:C6     | 2.41                     | 0.54              |
| 1:CA:1476:A:H2'   | 1:CA:1477:U:O4'    | 2.07                     | 0.54              |
| 5:CF:86:ARG:HH11  | 17:CR:63:TYR:HB3   | 1.72                     | 0.54              |
| 5:CF:92:THR:HG22  | 5:CF:93:LYS:H      | 1.73                     | 0.54              |
| 20:CB:76:SER:O    | 20:CB:80:LYS:HG2   | 2.06                     | 0.54              |
| 23:DB:20:C:H2'    | 23:DB:21:A:H8      | 1.72                     | 0.54              |
| 23:DB:184:C:H2'   | 23:DB:185:G:H8     | 1.71                     | 0.54              |
| 23:DB:554:U:H2'   | 23:DB:555:G:O4'    | 2.08                     | 0.54              |
| 23:DB:593:U:H2'   | 23:DB:594:U:C6     | 2.42                     | 0.54              |
| 23:DB:611:C:H2'   | 23:DB:612:G:O4'    | 2.07                     | 0.54              |
| 23:DB:696:G:O2'   | 23:DB:697:G:H5'    | 2.07                     | 0.54              |
| 23:DB:1005:C:H2'  | 23:DB:1006:C:H6    | 1.72                     | 0.54              |
| 23:DB:1083:U:H1'  | 23:DB:1086:A:N6    | 2.22                     | 0.54              |
| 23:DB:1259:G:H2'  | 23:DB:1260:A:H8    | 1.73                     | 0.54              |
| 23:DB:1637:A:H2'  | 23:DB:1638:C:H6    | 1.72                     | 0.54              |
| 23:DB:1904:G:O2'  | 23:DB:1905:C:H5'   | 2.07                     | 0.54              |
| 29:DG:29:ASN:HB2  | 29:DG:78:VAL:O     | 2.08                     | 0.54              |
| 30:DH:2:GLN:HB2   | 30:DH:19:VAL:HA    | 1.89                     | 0.54              |
| 30:DH:87:GLU:HB2  | 30:DH:89:LYS:HZ2   | 1.71                     | 0.54              |
| 31:DJ:37:ARG:CZ   | 31:DJ:110:PRO:HG3  | 2.37                     | 0.54              |
| 31:DJ:133:ALA:C   | 31:DJ:135:GLN:N    | 2.65                     | 0.54              |
| 33:DL:58:TYR:HA   | 33:DL:62:PRO:HD3   | 1.89                     | 0.54              |
| 34:DM:43:ALA:HB2  | 34:DM:69:PRO:HG3   | 1.89                     | 0.54              |
| 41:DT:66:LYS:HD2  | 41:DT:67:VAL:N     | 2.22                     | 0.54              |
| 44:DX:22:LEU:HD22 | 44:DX:25:GLN:OE1   | 2.07                     | 0.54              |
| 46:DZ:47:LYS:HD2  | 46:DZ:52:ALA:HA    | 1.89                     | 0.54              |
| 47:D0:52:LYS:HE2  | 47:D0:53:VAL:HB    | 1.89                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:235:C:H2'     | 1:AA:236:A:C8      | 2.43                     | 0.54              |
| 1:AA:777:A:H2'     | 1:AA:778:G:H8      | 1.72                     | 0.54              |
| 1:AA:971:G:OP1     | 1:AA:971:G:H3'     | 2.07                     | 0.54              |
| 2:AC:149:LYS:HB3   | 2:AC:200:TRP:HB2   | 1.90                     | 0.54              |
| 6:AG:67:ASN:ND2    | 6:AG:127:ALA:HA    | 2.20                     | 0.54              |
| 8:AI:17:ARG:O      | 8:AI:64:ILE:HA     | 2.08                     | 0.54              |
| 11:AL:87:LYS:HA    | 11:AL:87:LYS:NZ    | 2.21                     | 0.54              |
| 12:AM:5:GLY:O      | 12:AM:6:ILE:HG12   | 2.07                     | 0.54              |
| 12:AM:38:ILE:HG13  | 12:AM:55:LEU:HD21  | 1.89                     | 0.54              |
| 13:AN:30:ILE:HG21  | 13:AN:44:VAL:HG21  | 1.89                     | 0.54              |
| 13:AN:79:SER:O     | 13:AN:81:ILE:HD12  | 2.07                     | 0.54              |
| 15:AP:31:ARG:HG3   | 15:AP:31:ARG:HH11  | 1.72                     | 0.54              |
| 20:AB:173:LYS:HD3  | 20:AB:173:LYS:C    | 2.32                     | 0.54              |
| 20:AB:186:VAL:HG22 | 20:AB:198:VAL:HG23 | 1.89                     | 0.54              |
| 23:BB:288:U:O2'    | 23:BB:289:G:H5'    | 2.08                     | 0.54              |
| 23:BB:633:A:C2'    | 23:BB:634:C:H5'    | 2.37                     | 0.54              |
| 23:BB:802:A:H4'    | 55:BB:3474:HOH:O   | 2.08                     | 0.54              |
| 23:BB:1121:C:H2'   | 23:BB:1122:G:O4'   | 2.07                     | 0.54              |
| 23:BB:1480:C:H2'   | 23:BB:1481:U:C6    | 2.42                     | 0.54              |
| 23:BB:1819:A:OP1   | 25:BC:153:LEU:HB2  | 2.08                     | 0.54              |
| 23:BB:1821:A:H5'   | 25:BC:155:ARG:NH2  | 2.22                     | 0.54              |
| 23:BB:2398:U:H2'   | 23:BB:2399:G:C8    | 2.42                     | 0.54              |
| 23:BB:2527:C:H1'   | 51:B4:1:MET:CB     | 2.38                     | 0.54              |
| 23:BB:2840:C:H2'   | 23:BB:2841:C:H6    | 1.72                     | 0.54              |
| 25:BC:119:VAL:HG22 | 25:BC:130:PRO:HG2  | 1.89                     | 0.54              |
| 26:BD:52:THR:HG22  | 26:BD:76:GLY:N     | 2.23                     | 0.54              |
| 27:BE:141:MET:O    | 27:BE:143:LEU:HD22 | 2.08                     | 0.54              |
| 31:BJ:15:TRP:HA    | 31:BJ:53:TYR:O     | 2.07                     | 0.54              |
| 33:BL:82:LEU:C     | 33:BL:86:GLU:HG3   | 2.33                     | 0.54              |
| 39:BR:5:PHE:HA     | 39:BR:40:MET:HG2   | 1.88                     | 0.54              |
| 40:BS:38:TYR:CZ    | 47:B0:37:HIS:HA    | 2.42                     | 0.54              |
| 43:BW:47:GLY:O     | 43:BW:54:ARG:HA    | 2.08                     | 0.54              |
| 49:B2:44:VAL:HG23  | 49:B2:45:SER:N     | 2.16                     | 0.54              |
| 1:CA:22:G:H2'      | 1:CA:23:C:H6       | 1.73                     | 0.54              |
| 1:CA:1131:G:C2'    | 1:CA:1132:C:H5'    | 2.36                     | 0.54              |
| 1:CA:1524:C:H2'    | 1:CA:1525:G:C8     | 2.43                     | 0.54              |
| 12:CM:79:LEU:HD12  | 12:CM:80:MET:N     | 2.22                     | 0.54              |
| 19:CT:2:ASN:O      | 19:CT:4:LYS:N      | 2.40                     | 0.54              |
| 20:CB:96:LEU:HB2   | 20:CB:99:MET:CG    | 2.38                     | 0.54              |
| 23:DB:136:G:H2'    | 23:DB:137:U:H6     | 1.69                     | 0.54              |
| 23:DB:1430:G:H2'   | 23:DB:1431:A:C8    | 2.43                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DB:1488:C:O2'   | 23:DB:1489:C:H5'  | 2.08                     | 0.54              |
| 23:DB:1796:U:H2'   | 23:DB:1797:G:H8   | 1.73                     | 0.54              |
| 23:DB:2271:G:O2'   | 23:DB:2272:U:H5'  | 2.07                     | 0.54              |
| 26:DD:35:THR:HB    | 26:DD:48:ILE:CB   | 2.36                     | 0.54              |
| 26:DD:184:ARG:HD2  | 37:DP:4:ILE:CG2   | 2.38                     | 0.54              |
| 28:DF:41:GLU:O     | 28:DF:42:ALA:C    | 2.50                     | 0.54              |
| 32:DK:115:ILE:HG23 | 32:DK:116:ILE:N   | 2.22                     | 0.54              |
| 36:DO:18:LEU:HD13  | 43:DW:76:ARG:HH21 | 1.73                     | 0.54              |
| 36:DO:90:VAL:HG12  | 36:DO:91:SER:N    | 2.23                     | 0.54              |
| 39:DR:41:ILE:HG23  | 39:DR:43:ASN:HB2  | 1.88                     | 0.54              |
| 43:DW:19:ARG:HB2   | 43:DW:19:ARG:CZ   | 2.37                     | 0.54              |
| 43:DW:56:HIS:CD2   | 43:DW:57:THR:H    | 2.24                     | 0.54              |
| 44:DX:1:MET:CB     | 44:DX:6:LEU:HG    | 2.37                     | 0.54              |
| 45:DY:2:LYS:H      | 45:DY:37:ARG:CB   | 2.20                     | 0.54              |
| 1:AA:230:G:O2'     | 1:AA:231:U:H5'    | 2.07                     | 0.54              |
| 1:AA:936:C:H1'     | 1:AA:1382:C:H42   | 1.72                     | 0.54              |
| 1:AA:1220:G:H2'    | 1:AA:1221:G:H8    | 1.72                     | 0.54              |
| 1:AA:1380:U:O4     | 6:AG:2:ARG:HA     | 2.07                     | 0.54              |
| 2:AC:46:LEU:HD11   | 2:AC:86:LEU:HD21  | 1.90                     | 0.54              |
| 2:AC:78:LYS:CG     | 2:AC:81:GLU:HB2   | 2.34                     | 0.54              |
| 4:AE:156:ARG:HD3   | 7:AH:42:GLU:O     | 2.07                     | 0.54              |
| 8:AI:38:PHE:O      | 8:AI:44:ARG:HG2   | 2.08                     | 0.54              |
| 8:AI:99:LYS:HD3    | 8:AI:100:ALA:N    | 2.21                     | 0.54              |
| 15:AP:8:ARG:HE     | 15:AP:15:PRO:HB3  | 1.72                     | 0.54              |
| 15:AP:33:ILE:HD12  | 15:AP:33:ILE:N    | 2.21                     | 0.54              |
| 23:BB:272:A:H2'    | 23:BB:273:G:H8    | 1.72                     | 0.54              |
| 23:BB:445:C:H5'    | 27:BE:47:LYS:HZ3  | 1.70                     | 0.54              |
| 23:BB:611:C:H2'    | 23:BB:612:G:O4'   | 2.07                     | 0.54              |
| 23:BB:926:G:H2'    | 23:BB:927:A:C8    | 2.42                     | 0.54              |
| 23:BB:1024:G:C3'   | 23:BB:1025:G:H5'' | 2.34                     | 0.54              |
| 23:BB:1166:G:H2'   | 23:BB:1167:C:H6   | 1.73                     | 0.54              |
| 23:BB:1639:C:H2'   | 23:BB:1640:A:C5'  | 2.33                     | 0.54              |
| 23:BB:2843:G:O2'   | 23:BB:2844:G:H5'  | 2.08                     | 0.54              |
| 26:BD:12:THR:OG1   | 26:BD:14:ILE:HG12 | 2.06                     | 0.54              |
| 29:BG:172:GLU:O    | 29:BG:173:ALA:HB2 | 2.07                     | 0.54              |
| 36:BO:16:ARG:HG3   | 36:BO:20:GLU:HG3  | 1.90                     | 0.54              |
| 40:BS:29:VAL:HG21  | 40:BS:69:LEU:C    | 2.33                     | 0.54              |
| 44:BX:23:ARG:HH21  | 44:BX:27:ASN:CG   | 2.15                     | 0.54              |
| 52:BI:23:VAL:HG23  | 52:BI:24:GLY:H    | 1.71                     | 0.54              |
| 1:CA:128:G:H2'     | 1:CA:129:A:C8     | 2.43                     | 0.54              |
| 1:CA:173:U:H5'     | 1:CA:197:A:O4'    | 2.07                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:415:A:H3'    | 1:CA:416:G:H8     | 1.73                     | 0.54              |
| 1:CA:499:A:H4'    | 1:CA:500:G:OP1    | 2.06                     | 0.54              |
| 1:CA:979:C:H2'    | 1:CA:980:C:O4'    | 2.07                     | 0.54              |
| 1:CA:1030:U:O2'   | 1:CA:1031:C:P     | 2.65                     | 0.54              |
| 1:CA:1118:U:O2'   | 1:CA:1119:C:H5'   | 2.07                     | 0.54              |
| 1:CA:1216:A:H5''  | 13:CN:4:SER:HB2   | 1.90                     | 0.54              |
| 3:CD:160:LEU:HD22 | 3:CD:160:LEU:O    | 2.07                     | 0.54              |
| 5:CF:6:ILE:HD12   | 5:CF:7:VAL:N      | 2.22                     | 0.54              |
| 8:CI:51:LEU:HB3   | 8:CI:56:MET:CG    | 2.34                     | 0.54              |
| 9:CJ:37:ARG:NE    | 9:CJ:37:ARG:C     | 2.66                     | 0.54              |
| 9:CJ:65:TYR:HE1   | 13:CN:84:ARG:HA   | 1.72                     | 0.54              |
| 9:CJ:65:TYR:OH    | 13:CN:84:ARG:HG3  | 2.07                     | 0.54              |
| 11:CL:49:ARG:CG   | 11:CL:89:LEU:HD21 | 2.36                     | 0.54              |
| 15:CP:40:ASN:ND2  | 15:CP:42:ILE:HG12 | 2.22                     | 0.54              |
| 21:CU:4:LYS:HB3   | 21:CU:6:ARG:NH1   | 2.12                     | 0.54              |
| 23:DB:70:G:H3'    | 23:DB:113:U:H4'   | 1.89                     | 0.54              |
| 23:DB:354:A:H2'   | 23:DB:355:U:H6    | 1.69                     | 0.54              |
| 23:DB:512:G:OP1   | 23:DB:512:G:H4'   | 2.07                     | 0.54              |
| 23:DB:580:U:H2'   | 23:DB:581:C:H6    | 1.70                     | 0.54              |
| 23:DB:607:U:O4    | 23:DB:620:G:H5''  | 2.07                     | 0.54              |
| 23:DB:851:C:H2'   | 23:DB:852:U:H6    | 1.73                     | 0.54              |
| 23:DB:1287:A:O2'  | 23:DB:1288:G:H5'  | 2.08                     | 0.54              |
| 23:DB:1480:C:H2'  | 23:DB:1481:U:C6   | 2.43                     | 0.54              |
| 23:DB:2070:A:H2'  | 23:DB:2071:A:C8   | 2.43                     | 0.54              |
| 23:DB:2398:U:H2'  | 23:DB:2399:G:C8   | 2.42                     | 0.54              |
| 23:DB:2405:G:H4'  | 33:DL:70:LYS:HE3  | 1.90                     | 0.54              |
| 23:DB:2556:C:H2'  | 23:DB:2557:G:O4'  | 2.08                     | 0.54              |
| 23:DB:2839:G:H4'  | 35:DN:49:GLU:CG   | 2.30                     | 0.54              |
| 26:DD:83:ARG:O    | 26:DD:84:LEU:HB2  | 2.07                     | 0.54              |
| 27:DE:75:SER:OG   | 27:DE:77:ILE:HG22 | 2.07                     | 0.54              |
| 33:DL:92:LEU:HA   | 33:DL:96:LYS:CD   | 2.37                     | 0.54              |
| 41:DT:15:HIS:H    | 41:DT:32:LEU:HA   | 1.73                     | 0.54              |
| 1:AA:454:G:O2'    | 1:AA:455:G:H5'    | 2.07                     | 0.54              |
| 2:AC:96:VAL:HB    | 2:AC:97:PRO:HD2   | 1.88                     | 0.54              |
| 2:AC:183:TYR:HA   | 2:AC:199:VAL:O    | 2.07                     | 0.54              |
| 3:AD:25:ARG:NH1   | 3:AD:30:LYS:HG2   | 2.23                     | 0.54              |
| 9:AJ:88:MET:C     | 9:AJ:90:LEU:H     | 2.13                     | 0.54              |
| 13:AN:30:ILE:H    | 13:AN:30:ILE:CD1  | 2.18                     | 0.54              |
| 13:AN:66:THR:HG23 | 13:AN:67:GLY:N    | 2.22                     | 0.54              |
| 20:AB:53:LEU:HD21 | 20:AB:212:TYR:CE2 | 2.42                     | 0.54              |
| 22:BA:15:A:H1'    | 22:BA:109:A:C8    | 2.43                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:36:G:H2'    | 23:BB:37:C:O4'     | 2.08                     | 0.54              |
| 23:BB:233:A:N6    | 23:BB:428:A:H61    | 2.06                     | 0.54              |
| 23:BB:250:G:OP2   | 50:B3:7:ARG:HD3    | 2.08                     | 0.54              |
| 23:BB:480:A:H4'   | 42:BU:42:LYS:CG    | 2.32                     | 0.54              |
| 23:BB:649:G:N2    | 50:B3:44:ARG:HH22  | 2.06                     | 0.54              |
| 23:BB:705:A:H61   | 23:BB:726:G:H1'    | 1.73                     | 0.54              |
| 23:BB:718:A:H3'   | 23:BB:719:C:C6     | 2.41                     | 0.54              |
| 23:BB:877:A:C2    | 23:BB:900:A:N7     | 2.76                     | 0.54              |
| 23:BB:1013:C:H2'  | 23:BB:1014:A:C8    | 2.42                     | 0.54              |
| 23:BB:1097:U:C2'  | 23:BB:1098:A:H5'   | 2.36                     | 0.54              |
| 23:BB:1559:U:H3'  | 23:BB:1560:G:H5'   | 1.88                     | 0.54              |
| 23:BB:1667:G:OP1  | 32:BK:6:THR:HA     | 2.07                     | 0.54              |
| 23:BB:1946:U:H2'  | 23:BB:1947:C:C6    | 2.43                     | 0.54              |
| 23:BB:2218:G:H2'  | 23:BB:2219:U:C6    | 2.43                     | 0.54              |
| 23:BB:2484:G:HO2' | 34:BM:45:GLN:CD    | 2.15                     | 0.54              |
| 23:BB:2556:C:H2'  | 23:BB:2557:G:O4'   | 2.08                     | 0.54              |
| 23:BB:2704:C:H2'  | 23:BB:2705:A:O4'   | 2.07                     | 0.54              |
| 25:BC:124:LYS:O   | 25:BC:191:LEU:HD13 | 2.07                     | 0.54              |
| 30:BH:73:ASN:HD22 | 30:BH:74:ALA:H     | 1.55                     | 0.54              |
| 35:BN:29:VAL:HB   | 35:BN:75:ILE:HG12  | 1.89                     | 0.54              |
| 36:BO:41:ALA:HB3  | 36:BO:45:SER:O     | 2.07                     | 0.54              |
| 38:BQ:88:GLU:HA   | 39:BR:53:PHE:CE1   | 2.42                     | 0.54              |
| 41:BT:30:ILE:CG2  | 41:BT:31:VAL:N     | 2.70                     | 0.54              |
| 42:BU:33:VAL:HG12 | 42:BU:35:VAL:CG2   | 2.38                     | 0.54              |
| 47:B0:42:ILE:HG12 | 47:B0:43:THR:N     | 2.22                     | 0.54              |
| 1:CA:108:G:C6     | 19:CT:9:ARG:HG2    | 2.41                     | 0.54              |
| 1:CA:266:G:HO2'   | 1:CA:267:C:H3'     | 1.73                     | 0.54              |
| 1:CA:337:G:H2'    | 1:CA:338:A:C8      | 2.43                     | 0.54              |
| 1:CA:539:A:H2'    | 1:CA:540:G:H8      | 1.73                     | 0.54              |
| 1:CA:777:A:H2'    | 1:CA:778:G:H8      | 1.72                     | 0.54              |
| 1:CA:930:C:H2'    | 1:CA:931:C:C6      | 2.41                     | 0.54              |
| 3:CD:2:ARG:HA     | 3:CD:2:ARG:HE      | 1.73                     | 0.54              |
| 3:CD:55:ARG:HG3   | 3:CD:55:ARG:NH1    | 2.20                     | 0.54              |
| 3:CD:151:GLN:HE21 | 3:CD:153:ARG:HD2   | 1.73                     | 0.54              |
| 6:CG:22:LEU:O     | 6:CG:26:VAL:HG13   | 2.06                     | 0.54              |
| 6:CG:136:LYS:O    | 6:CG:140:VAL:HG23  | 2.07                     | 0.54              |
| 20:CB:86:CYS:HB3  | 20:CB:88:GLN:HG3   | 1.90                     | 0.54              |
| 20:CB:96:LEU:HD12 | 20:CB:99:MET:HE3   | 1.90                     | 0.54              |
| 22:DA:102:G:H2'   | 22:DA:103:U:H6     | 1.72                     | 0.54              |
| 23:DB:95:A:O2'    | 44:DX:41:HIS:HA    | 2.08                     | 0.54              |
| 23:DB:160:A:H2'   | 23:DB:161:A:C8     | 2.42                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DB:431:U:O2'    | 23:DB:432:A:H5'   | 2.08                     | 0.54              |
| 23:DB:535:G:O2'    | 23:DB:536:G:H5'   | 2.08                     | 0.54              |
| 23:DB:1168:G:O2'   | 23:DB:1169:A:H5'  | 2.07                     | 0.54              |
| 23:DB:1487:U:H2'   | 23:DB:1488:C:H6   | 1.73                     | 0.54              |
| 23:DB:1591:A:H2'   | 23:DB:1592:C:C6   | 2.42                     | 0.54              |
| 23:DB:2025:C:P     | 26:DD:154:LYS:HE3 | 2.47                     | 0.54              |
| 26:DD:60:VAL:HG23  | 26:DD:63:PRO:CG   | 2.33                     | 0.54              |
| 34:DM:96:ILE:HG22  | 34:DM:97:GLN:NE2  | 2.22                     | 0.54              |
| 39:DR:37:GLU:HG2   | 39:DR:62:GLU:C    | 2.33                     | 0.54              |
| 39:DR:40:MET:CG    | 39:DR:54:VAL:HG13 | 2.36                     | 0.54              |
| 44:DX:17:GLU:CD    | 44:DX:17:GLU:H    | 2.14                     | 0.54              |
| 52:DI:5:GLN:O      | 52:DI:6:ALA:HB3   | 2.07                     | 0.54              |
| 1:AA:405:U:O4      | 3:AD:1:ALA:HA     | 2.07                     | 0.54              |
| 1:AA:1281:C:H5'    | 1:AA:1282:C:H5    | 1.73                     | 0.54              |
| 1:AA:1391:U:H2'    | 1:AA:1392:G:H8    | 1.72                     | 0.54              |
| 1:AA:1452:C:H4'    | 1:AA:1453:G:C5'   | 2.37                     | 0.54              |
| 1:AA:1527:U:O2'    | 1:AA:1528:U:H5'   | 2.07                     | 0.54              |
| 2:AC:40:GLN:NE2    | 2:AC:44:LYS:HD2   | 2.22                     | 0.54              |
| 8:AI:56:MET:HE2    | 8:AI:57:VAL:H     | 1.72                     | 0.54              |
| 11:AL:106:VAL:CG2  | 11:AL:116:TYR:HB3 | 2.38                     | 0.54              |
| 15:AP:46:LYS:H     | 15:AP:46:LYS:HD3  | 1.73                     | 0.54              |
| 19:AT:49:ALA:O     | 19:AT:52:GLU:HB3  | 2.08                     | 0.54              |
| 23:BB:533:G:H5'    | 38:BQ:23:TYR:CD1  | 2.43                     | 0.54              |
| 23:BB:770:G:O2'    | 23:BB:771:G:H5'   | 2.07                     | 0.54              |
| 23:BB:1210:G:H5''  | 23:BB:1211:C:O5'  | 2.07                     | 0.54              |
| 23:BB:1430:G:H2'   | 23:BB:1431:A:C8   | 2.43                     | 0.54              |
| 23:BB:1593:A:H2'   | 23:BB:1594:U:C6   | 2.42                     | 0.54              |
| 24:BV:63:ILE:O     | 24:BV:65:VAL:HG22 | 2.07                     | 0.54              |
| 25:BC:67:LYS:CG    | 25:BC:68:ARG:H    | 2.14                     | 0.54              |
| 25:BC:141:HIS:CG   | 25:BC:190:THR:HB  | 2.42                     | 0.54              |
| 26:BD:58:ASN:O     | 26:BD:59:ARG:HB2  | 2.07                     | 0.54              |
| 26:BD:128:ARG:HD3  | 26:BD:142:VAL:O   | 2.08                     | 0.54              |
| 27:BE:43:THR:O     | 27:BE:89:PRO:HA   | 2.07                     | 0.54              |
| 28:BF:71:LYS:HD3   | 28:BF:71:LYS:C    | 2.32                     | 0.54              |
| 30:BH:83:LYS:HG3   | 1:CA:360:G:OP1    | 2.07                     | 0.54              |
| 31:BJ:41:LYS:O     | 38:BQ:66:ALA:HB1  | 2.08                     | 0.54              |
| 32:BK:119:ALA:N    | 32:BK:120:PRO:HD3 | 2.23                     | 0.54              |
| 33:BL:117:THR:HG21 | 33:BL:120:VAL:CB  | 2.37                     | 0.54              |
| 34:BM:73:ILE:HD11  | 34:BM:92:TRP:HB2  | 1.89                     | 0.54              |
| 35:BN:12:ARG:HD3   | 35:BN:20:MET:HG3  | 1.90                     | 0.54              |
| 35:BN:34:ILE:HG12  | 35:BN:34:ILE:O    | 2.07                     | 0.54              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BN:83:LEU:HA    | 35:BN:86:ARG:HD3   | 1.88                     | 0.54              |
| 36:BO:91:SER:HB2   | 36:BO:115:LEU:HG   | 1.89                     | 0.54              |
| 37:BP:61:ARG:NH2   | 37:BP:75:THR:HB    | 2.22                     | 0.54              |
| 40:BS:86:MET:HB2   | 40:BS:96:ILE:CD1   | 2.38                     | 0.54              |
| 41:BT:84:TYR:O     | 41:BT:85:VAL:HG22  | 2.08                     | 0.54              |
| 48:B1:9:LYS:HG2    | 50:B3:34:LYS:NZ    | 2.23                     | 0.54              |
| 1:CA:476:U:H2'     | 1:CA:477:C:H6      | 1.73                     | 0.54              |
| 1:CA:766:A:H2      | 1:CA:1525:G:N3     | 2.06                     | 0.54              |
| 1:CA:1296:C:H4'    | 1:CA:1302:C:C4     | 2.43                     | 0.54              |
| 1:CA:1487:G:O2'    | 1:CA:1488:G:H5'    | 2.07                     | 0.54              |
| 2:CC:51:VAL:HG11   | 2:CC:67:ILE:HD11   | 1.89                     | 0.54              |
| 3:CD:58:GLN:HA     | 3:CD:58:GLN:NE2    | 2.16                     | 0.54              |
| 3:CD:196:GLU:O     | 3:CD:199:ILE:HG23  | 2.06                     | 0.54              |
| 4:CE:19:ARG:CG     | 4:CE:20:VAL:H      | 2.13                     | 0.54              |
| 23:DB:26:G:H2'     | 23:DB:27:G:C1'     | 2.37                     | 0.54              |
| 23:DB:663:G:OP1    | 33:DL:27:LEU:HD13  | 2.08                     | 0.54              |
| 23:DB:2666:C:O4'   | 23:DB:2666:C:O2    | 2.24                     | 0.54              |
| 23:DB:2692:G:O2'   | 23:DB:2693:G:H5'   | 2.07                     | 0.54              |
| 23:DB:2704:C:H2'   | 23:DB:2705:A:O4'   | 2.07                     | 0.54              |
| 23:DB:2849:U:H4'   | 23:DB:2850:A:C5'   | 2.37                     | 0.54              |
| 27:DE:77:ILE:HG23  | 27:DE:78:TRP:HD1   | 1.73                     | 0.54              |
| 30:DH:75:LEU:HD23  | 30:DH:75:LEU:N     | 2.22                     | 0.54              |
| 35:DN:70:THR:HG22  | 35:DN:72:ASP:N     | 2.23                     | 0.54              |
| 37:DP:78:PRO:O     | 37:DP:79:VAL:HG22  | 2.07                     | 0.54              |
| 43:DW:4:LYS:HZ2    | 43:DW:4:LYS:H      | 1.54                     | 0.54              |
| 1:AA:1244:G:H2'    | 1:AA:1245:C:H6     | 1.73                     | 0.54              |
| 3:AD:18:LEU:HD22   | 3:AD:63:ILE:HG12   | 1.90                     | 0.54              |
| 5:AF:18:VAL:N      | 5:AF:19:PRO:HD2    | 2.22                     | 0.54              |
| 9:AJ:88:MET:HE3    | 9:AJ:88:MET:H      | 1.73                     | 0.54              |
| 23:BB:329:G:H1     | 42:BU:16:LYS:HD3   | 1.73                     | 0.54              |
| 23:BB:425:G:H2'    | 23:BB:426:C:H6     | 1.72                     | 0.54              |
| 23:BB:581:C:H2'    | 23:BB:582:A:C8     | 2.43                     | 0.54              |
| 23:BB:615:U:C2     | 27:BE:38:GLY:HA3   | 2.42                     | 0.54              |
| 23:BB:741:U:H2'    | 23:BB:742:A:C8     | 2.42                     | 0.54              |
| 23:BB:751:A:H5'    | 40:BS:90:LYS:CE    | 2.38                     | 0.54              |
| 23:BB:936:A:H2'    | 23:BB:937:C:H6     | 1.71                     | 0.54              |
| 23:BB:1816:C:C5    | 25:BC:62:ARG:HD2   | 2.42                     | 0.54              |
| 23:BB:1917:U:C2'   | 23:BB:1918:A:H5'   | 2.37                     | 0.54              |
| 25:BC:124:LYS:CB   | 25:BC:125:PRO:CD   | 2.83                     | 0.54              |
| 26:BD:131:ASP:O    | 26:BD:139:SER:HA   | 2.08                     | 0.54              |
| 26:BD:175:LEU:HD13 | 26:BD:189:VAL:HG11 | 1.90                     | 0.54              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BE:119:ILE:HD12 | 27:BE:119:ILE:N    | 2.23                     | 0.54              |
| 30:BH:83:LYS:HB2   | 30:BH:92:GLY:N     | 2.23                     | 0.54              |
| 30:BH:114:GLU:OE2  | 30:BH:134:VAL:HG23 | 2.07                     | 0.54              |
| 33:BL:38:GLN:H     | 33:BL:41:ARG:HH11  | 1.56                     | 0.54              |
| 33:BL:82:LEU:O     | 33:BL:117:THR:HG22 | 2.06                     | 0.54              |
| 35:BN:120:GLU:C    | 35:BN:121:LYS:HD2  | 2.32                     | 0.54              |
| 39:BR:47:VAL:HG22  | 39:BR:48:LYS:N     | 2.19                     | 0.54              |
| 50:B3:59:ALA:O     | 50:B3:60:CYS:HB2   | 2.07                     | 0.54              |
| 51:B4:24:ARG:HG3   | 51:B4:24:ARG:HH11  | 1.73                     | 0.54              |
| 1:CA:34:C:H2'      | 1:CA:35:G:C8       | 2.42                     | 0.54              |
| 1:CA:231:U:P       | 15:CP:31:ARG:HH12  | 2.31                     | 0.54              |
| 1:CA:235:C:H2'     | 1:CA:236:A:C8      | 2.43                     | 0.54              |
| 1:CA:719:C:H1'     | 17:CR:37:LYS:CB    | 2.32                     | 0.54              |
| 3:CD:127:ARG:HD2   | 3:CD:127:ARG:H     | 1.73                     | 0.54              |
| 8:CI:51:LEU:HD13   | 8:CI:56:MET:SD     | 2.48                     | 0.54              |
| 13:CN:26:LEU:HD21  | 13:CN:47:LEU:HG    | 1.90                     | 0.54              |
| 13:CN:30:ILE:O     | 13:CN:44:VAL:HB    | 2.07                     | 0.54              |
| 20:CB:57:ASN:HD22  | 20:CB:223:GLY:HA2  | 1.73                     | 0.54              |
| 23:DB:96:C:OP1     | 44:DX:41:HIS:HB2   | 2.08                     | 0.54              |
| 23:DB:323:C:O2'    | 27:DE:163:ASN:C    | 2.50                     | 0.54              |
| 23:DB:533:G:H2'    | 23:DB:534:U:H6     | 1.73                     | 0.54              |
| 23:DB:1387:A:H2'   | 23:DB:1388:G:C8    | 2.42                     | 0.54              |
| 23:DB:1593:A:H2'   | 23:DB:1594:U:C6    | 2.42                     | 0.54              |
| 23:DB:1723:G:N7    | 23:DB:1737:G:N2    | 2.56                     | 0.54              |
| 23:DB:2213:U:O2    | 23:DB:2213:U:C2'   | 2.55                     | 0.54              |
| 23:DB:2247:A:H2'   | 23:DB:2248:C:C6    | 2.43                     | 0.54              |
| 23:DB:2257:U:C5'   | 43:DW:5:ALA:HB2    | 2.37                     | 0.54              |
| 23:DB:2657:A:H2'   | 23:DB:2658:C:O4'   | 2.07                     | 0.54              |
| 24:DV:53:LYS:HB3   | 24:DV:53:LYS:NZ    | 2.23                     | 0.54              |
| 27:DE:102:ARG:HA   | 27:DE:105:LEU:HD23 | 1.90                     | 0.54              |
| 27:DE:148:ILE:CA   | 27:DE:185:LYS:HB3  | 2.32                     | 0.54              |
| 27:DE:149:ILE:O    | 27:DE:149:ILE:HG13 | 2.08                     | 0.54              |
| 28:DF:141:ASP:HB3  | 28:DF:143:ASP:OD1  | 2.07                     | 0.54              |
| 31:DJ:35:ARG:HH22  | 31:DJ:41:LYS:H     | 1.54                     | 0.54              |
| 31:DJ:105:VAL:HG11 | 31:DJ:122:LEU:HD11 | 1.89                     | 0.54              |
| 33:DL:47:ARG:O     | 33:DL:48:ARG:HD3   | 2.08                     | 0.54              |
| 34:DM:91:TYR:N     | 34:DM:91:TYR:CD2   | 2.74                     | 0.54              |
| 36:DO:26:LEU:O     | 36:DO:40:ILE:HD11  | 2.06                     | 0.54              |
| 37:DP:109:ILE:O    | 37:DP:111:GLU:N    | 2.40                     | 0.54              |
| 38:DQ:39:ILE:HA    | 38:DQ:43:GLN:HE21  | 1.72                     | 0.54              |
| 41:DT:92:ASN:C     | 41:DT:93:LEU:HD12  | 2.32                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 43:DW:19:ARG:HH21 | 43:DW:22:VAL:HA    | 1.73                     | 0.54              |
| 46:DZ:14:ALA:HA   | 46:DZ:24:ILE:HA    | 1.89                     | 0.54              |
| 52:DI:121:ILE:H   | 52:DI:121:ILE:CD1  | 2.18                     | 0.54              |
| 1:AA:255:G:H5'    | 16:AQ:17:GLU:O     | 2.08                     | 0.54              |
| 1:AA:764:C:H2'    | 1:AA:765:G:H5'     | 1.88                     | 0.54              |
| 1:AA:1244:G:H2'   | 1:AA:1245:C:C6     | 2.43                     | 0.54              |
| 1:AA:1306:A:N6    | 1:AA:1331:G:H1'    | 2.23                     | 0.54              |
| 1:AA:1477:U:H2'   | 1:AA:1478:U:C6     | 2.43                     | 0.54              |
| 12:AM:2:ARG:HG3   | 12:AM:8:ILE:HG23   | 1.89                     | 0.54              |
| 13:AN:19:TYR:HD2  | 13:AN:23:ARG:HD3   | 1.73                     | 0.54              |
| 23:BB:7:G:H2'     | 23:BB:8:C:O4'      | 2.08                     | 0.54              |
| 23:BB:139:U:C4    | 41:BT:1:MET:HB2    | 2.42                     | 0.54              |
| 23:BB:438:G:H2'   | 23:BB:439:A:C8     | 2.42                     | 0.54              |
| 23:BB:709:U:H2'   | 23:BB:710:U:C6     | 2.43                     | 0.54              |
| 23:BB:1723:G:N7   | 23:BB:1737:G:N2    | 2.56                     | 0.54              |
| 23:BB:2761:A:H1'  | 29:BG:142:GLN:NE2  | 2.23                     | 0.54              |
| 23:BB:2811:G:H5'  | 26:BD:62:LYS:HD2   | 1.88                     | 0.54              |
| 27:BE:180:LEU:HA  | 27:BE:186:VAL:HG21 | 1.88                     | 0.54              |
| 29:BG:84:LYS:NZ   | 29:BG:85:LYS:H     | 2.06                     | 0.54              |
| 29:BG:94:ARG:HH11 | 29:BG:94:ARG:CB    | 2.20                     | 0.54              |
| 29:BG:157:LYS:CG  | 29:BG:159:LYS:HZ2  | 2.20                     | 0.54              |
| 32:BK:98:ARG:HD2  | 32:BK:98:ARG:H     | 1.71                     | 0.54              |
| 33:BL:57:LEU:C    | 33:BL:59:ARG:H     | 2.13                     | 0.54              |
| 35:BN:116:VAL:O   | 35:BN:117:ASP:HB2  | 2.08                     | 0.54              |
| 39:BR:39:LEU:HD12 | 39:BR:60:LYS:N     | 2.23                     | 0.54              |
| 43:BW:80:SER:OG   | 43:BW:84:GLU:HB2   | 2.08                     | 0.54              |
| 46:BZ:30:HIS:O    | 46:BZ:31:ASP:HB3   | 2.07                     | 0.54              |
| 48:B1:26:LYS:HD3  | 48:B1:29:LYS:HB2   | 1.88                     | 0.54              |
| 1:CA:335:C:H2'    | 1:CA:336:A:H8      | 1.72                     | 0.54              |
| 1:CA:845:A:H3'    | 1:CA:846:G:O4'     | 2.08                     | 0.54              |
| 10:CK:83:VAL:HG21 | 10:CK:96:ILE:HG23  | 1.88                     | 0.54              |
| 23:DB:1439:A:C6   | 23:DB:1552:A:C5    | 2.95                     | 0.54              |
| 23:DB:1464:G:H2'  | 23:DB:1465:G:C8    | 2.43                     | 0.54              |
| 23:DB:1515:A:H5'  | 23:DB:1557:C:H5'   | 1.88                     | 0.54              |
| 23:DB:2020:A:H5'  | 47:D0:8:THR:HG23   | 1.90                     | 0.54              |
| 23:DB:2250:G:C6   | 34:DM:81:ARG:HG2   | 2.42                     | 0.54              |
| 23:DB:2386:A:H4'  | 43:DW:38:ARG:HB2   | 1.89                     | 0.54              |
| 23:DB:2649:C:H2'  | 23:DB:2650:U:H6    | 1.73                     | 0.54              |
| 24:DV:26:PHE:CE2  | 24:DV:44:HIS:HA    | 2.43                     | 0.54              |
| 26:DD:23:PRO:HA   | 26:DD:189:VAL:O    | 2.08                     | 0.54              |
| 27:DE:97:ASN:HB2  | 27:DE:100:MET:HB2  | 1.89                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:DJ:49:ASP:O    | 31:DJ:50:THR:CB    | 2.56                     | 0.54              |
| 38:DQ:2:ARG:HG2   | 38:DQ:4:LYS:HE3    | 1.89                     | 0.54              |
| 38:DQ:73:ILE:HG23 | 38:DQ:74:SER:N     | 2.22                     | 0.54              |
| 41:DT:55:VAL:HG21 | 41:DT:85:VAL:HB    | 1.89                     | 0.54              |
| 42:DU:9:GLU:HB2   | 42:DU:71:ILE:CG1   | 2.38                     | 0.54              |
| 42:DU:28:LEU:HD13 | 42:DU:30:SER:N     | 2.07                     | 0.54              |
| 52:DI:18:ASN:HB2  | 52:DI:38:CYS:SG    | 2.48                     | 0.54              |
| 52:DI:89:SER:HA   | 52:DI:97:VAL:HG11  | 1.90                     | 0.54              |
| 1:AA:337:G:H2'    | 1:AA:338:A:C8      | 2.43                     | 0.54              |
| 1:AA:399:G:H2'    | 1:AA:400:C:C6      | 2.42                     | 0.54              |
| 1:AA:472:U:H2'    | 1:AA:473:U:C6      | 2.43                     | 0.54              |
| 1:AA:1325:C:O2'   | 1:AA:1326:U:H5'    | 2.08                     | 0.54              |
| 3:AD:169:TRP:NE1  | 3:AD:170:LEU:HD23  | 2.22                     | 0.54              |
| 4:AE:35:LEU:HD23  | 4:AE:36:THR:N      | 2.23                     | 0.54              |
| 4:AE:131:ASN:O    | 4:AE:135:VAL:HG22  | 2.08                     | 0.54              |
| 12:AM:2:ARG:HD2   | 12:AM:2:ARG:N      | 2.23                     | 0.54              |
| 16:AQ:68:LYS:O    | 16:AQ:69:THR:CB    | 2.56                     | 0.54              |
| 23:BB:322:A:H5'   | 23:BB:340:A:C1'    | 2.38                     | 0.54              |
| 23:BB:433:C:O2'   | 23:BB:434:U:H5'    | 2.08                     | 0.54              |
| 23:BB:1061:U:H4'  | 23:BB:1070:A:O3'   | 2.08                     | 0.54              |
| 23:BB:1083:U:H2'  | 23:BB:1085:A:OP2   | 2.08                     | 0.54              |
| 23:BB:1171:G:H2'  | 23:BB:1172:C:C1'   | 2.38                     | 0.54              |
| 23:BB:1287:A:O2'  | 23:BB:1288:G:H5'   | 2.08                     | 0.54              |
| 23:BB:1400:U:H2'  | 23:BB:1401:G:C8    | 2.41                     | 0.54              |
| 23:BB:1413:A:H2'  | 23:BB:1414:C:C6    | 2.43                     | 0.54              |
| 23:BB:1716:U:H2'  | 23:BB:1717:A:C8    | 2.43                     | 0.54              |
| 23:BB:1745:A:H2'  | 23:BB:1746:A:H8    | 1.73                     | 0.54              |
| 23:BB:1797:G:OP1  | 25:BC:251:THR:HG23 | 2.08                     | 0.54              |
| 23:BB:1934:C:O2'  | 23:BB:1935:G:H5'   | 2.08                     | 0.54              |
| 23:BB:2489:U:O2'  | 23:BB:2490:G:H5'   | 2.08                     | 0.54              |
| 23:BB:2780:G:N1   | 31:BJ:120:ARG:HG3  | 2.22                     | 0.54              |
| 23:BB:2822:G:O6   | 35:BN:1:MET:N      | 2.41                     | 0.54              |
| 26:BD:34:VAL:HA   | 26:BD:89:GLU:CB    | 2.32                     | 0.54              |
| 28:BF:59:ILE:HD13 | 28:BF:59:ILE:O     | 2.08                     | 0.54              |
| 31:BJ:17:VAL:CG1  | 31:BJ:57:LEU:HD21  | 2.38                     | 0.54              |
| 32:BK:61:VAL:HG23 | 32:BK:84:CYS:O     | 2.08                     | 0.54              |
| 34:BM:59:ARG:HD2  | 34:BM:59:ARG:N     | 2.22                     | 0.54              |
| 35:BN:10:LEU:O    | 35:BN:12:ARG:N     | 2.40                     | 0.54              |
| 37:BP:23:ASP:HA   | 37:BP:48:ALA:O     | 2.08                     | 0.54              |
| 37:BP:99:LEU:HD21 | 37:BP:109:ILE:HG23 | 1.90                     | 0.54              |
| 38:BQ:52:ARG:NH2  | 38:BQ:55:GLN:HG2   | 2.23                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 44:BX:44:LYS:O    | 44:BX:44:LYS:HD2  | 2.08                     | 0.54              |
| 47:B0:36:LYS:HG3  | 47:B0:41:HIS:CA   | 2.38                     | 0.54              |
| 48:B1:26:LYS:HD3  | 48:B1:29:LYS:HD3  | 1.90                     | 0.54              |
| 52:BI:14:ALA:HB1  | 52:BI:50:LYS:HA   | 1.89                     | 0.54              |
| 1:CA:472:U:H2'    | 1:CA:473:U:C6     | 2.43                     | 0.54              |
| 1:CA:1135:U:H4'   | 1:CA:1136:C:OP1   | 2.05                     | 0.54              |
| 6:CG:110:ARG:HE   | 6:CG:122:GLU:HB2  | 1.72                     | 0.54              |
| 14:CO:80:LEU:HD21 | 14:CO:84:LEU:HD22 | 1.90                     | 0.54              |
| 18:CS:43:MET:C    | 18:CS:46:LEU:HD23 | 2.32                     | 0.54              |
| 19:CT:27:MET:HG2  | 19:CT:31:ILE:HD11 | 1.90                     | 0.54              |
| 23:DB:581:C:H2'   | 23:DB:582:A:C8    | 2.43                     | 0.54              |
| 23:DB:770:G:O2'   | 23:DB:771:G:H5'   | 2.08                     | 0.54              |
| 23:DB:1000:A:H2'  | 23:DB:1001:A:C8   | 2.43                     | 0.54              |
| 23:DB:1132:U:H5'' | 31:DJ:85:LYS:HD3  | 1.89                     | 0.54              |
| 23:DB:1219:U:H2'  | 23:DB:1220:G:H8   | 1.73                     | 0.54              |
| 23:DB:1671:U:H2'  | 23:DB:1673:G:OP2  | 2.08                     | 0.54              |
| 23:DB:1773:A:H62  | 25:DC:206:LYS:HE2 | 1.73                     | 0.54              |
| 23:DB:2387:U:O2'  | 43:DW:37:VAL:HG11 | 2.08                     | 0.54              |
| 23:DB:2405:G:H1'  | 23:DB:2412:A:N6   | 2.23                     | 0.54              |
| 23:DB:2557:G:H2'  | 23:DB:2558:C:H6   | 1.70                     | 0.54              |
| 23:DB:2741:A:H2'  | 23:DB:2742:G:O4'  | 2.08                     | 0.54              |
| 23:DB:2840:C:H2'  | 23:DB:2841:C:H6   | 1.72                     | 0.54              |
| 30:DH:82:SER:C    | 30:DH:83:LYS:HD2  | 2.33                     | 0.54              |
| 31:DJ:58:ASN:C    | 31:DJ:60:ASP:H    | 2.16                     | 0.54              |
| 32:DK:6:THR:HG22  | 32:DK:7:MET:N     | 2.23                     | 0.54              |
| 32:DK:24:VAL:HA   | 32:DK:39:ILE:CD1  | 2.38                     | 0.54              |
| 36:DO:82:ALA:O    | 36:DO:83:LEU:HD12 | 2.08                     | 0.54              |
| 37:DP:55:HIS:O    | 37:DP:57:ALA:N    | 2.38                     | 0.54              |
| 45:DY:1:ALA:O     | 45:DY:43:ILE:HG13 | 2.08                     | 0.54              |
| 48:D1:49:LYS:HZ2  | 48:D1:50:GLU:N    | 2.06                     | 0.54              |
| 52:DI:10:LEU:HD12 | 52:DI:10:LEU:O    | 2.08                     | 0.54              |
| 1:AA:22:G:H2'     | 1:AA:23:C:H6      | 1.73                     | 0.54              |
| 1:AA:177:G:H5''   | 19:AT:59:ARG:HH21 | 1.73                     | 0.54              |
| 1:AA:471:U:H2'    | 1:AA:472:U:H6     | 1.72                     | 0.54              |
| 1:AA:591:U:H2'    | 1:AA:592:G:H8     | 1.71                     | 0.54              |
| 1:AA:736:C:H2'    | 1:AA:737:C:C6     | 2.43                     | 0.54              |
| 1:AA:787:A:O2'    | 1:AA:788:U:H5'    | 2.08                     | 0.54              |
| 1:AA:1071:C:H2'   | 1:AA:1072:G:C8    | 2.40                     | 0.54              |
| 1:AA:1461:G:H2'   | 1:AA:1462:C:H6    | 1.69                     | 0.54              |
| 6:AG:14:ASP:OD1   | 6:AG:15:PRO:HD2   | 2.08                     | 0.54              |
| 16:AQ:74:LEU:HD22 | 16:AQ:75:VAL:N    | 2.22                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 20:AB:95:TRP:CE3  | 20:AB:171:ALA:HA   | 2.43                     | 0.54              |
| 22:BA:86:G:H2'    | 22:BA:87:U:O4'     | 2.08                     | 0.54              |
| 23:BB:331:C:O2'   | 23:BB:332:A:H5'    | 2.08                     | 0.54              |
| 23:BB:854:C:H2'   | 23:BB:855:G:C8     | 2.41                     | 0.54              |
| 23:BB:855:G:H21   | 43:BW:23:LYS:HB3   | 1.70                     | 0.54              |
| 23:BB:871:U:H2'   | 23:BB:872:U:C6     | 2.43                     | 0.54              |
| 23:BB:956:G:H5''  | 34:BM:76:LYS:HE2   | 1.89                     | 0.54              |
| 23:BB:992:C:O2'   | 23:BB:993:G:H5'    | 2.08                     | 0.54              |
| 23:BB:1149:G:H2'  | 23:BB:1150:C:C6    | 2.43                     | 0.54              |
| 23:BB:1432:G:O2'  | 23:BB:1433:A:H5'   | 2.07                     | 0.54              |
| 23:BB:1441:G:H2'  | 23:BB:1442:U:H6    | 1.73                     | 0.54              |
| 23:BB:1464:G:H2'  | 23:BB:1465:G:C8    | 2.43                     | 0.54              |
| 23:BB:1682:G:C2   | 23:BB:1757:A:O4'   | 2.61                     | 0.54              |
| 23:BB:1751:U:H2'  | 23:BB:1752:C:C6    | 2.43                     | 0.54              |
| 23:BB:2272:U:H3'  | 23:BB:2272:U:H6    | 1.73                     | 0.54              |
| 33:BL:60:ARG:C    | 50:B3:11:LYS:HZ3   | 2.16                     | 0.54              |
| 33:BL:119:PRO:O   | 33:BL:120:VAL:HB   | 2.06                     | 0.54              |
| 34:BM:96:ILE:HD13 | 34:BM:97:GLN:CB    | 2.38                     | 0.54              |
| 37:BP:32:VAL:HG13 | 37:BP:40:GLN:NE2   | 2.23                     | 0.54              |
| 41:BT:61:LEU:HD12 | 41:BT:62:VAL:N     | 2.22                     | 0.54              |
| 43:BW:43:LYS:O    | 43:BW:45:HIS:N     | 2.41                     | 0.54              |
| 46:BZ:49:ARG:HD3  | 46:BZ:50:ASP:N     | 2.22                     | 0.54              |
| 52:BI:124:MET:O   | 52:BI:128:ILE:HG12 | 2.08                     | 0.54              |
| 1:CA:44:A:O2'     | 1:CA:45:G:H5'      | 2.08                     | 0.54              |
| 1:CA:366:A:O2'    | 1:CA:367:U:OP1     | 2.24                     | 0.54              |
| 1:CA:600:A:H2'    | 1:CA:601:G:H8      | 1.73                     | 0.54              |
| 1:CA:1314:C:H2'   | 1:CA:1315:U:C6     | 2.43                     | 0.54              |
| 3:CD:115:GLN:NE2  | 3:CD:153:ARG:HH12  | 2.05                     | 0.54              |
| 4:CE:32:PHE:CE2   | 4:CE:55:VAL:HG22   | 2.43                     | 0.54              |
| 5:CF:18:VAL:HG21  | 5:CF:58:HIS:CE1    | 2.42                     | 0.54              |
| 8:CI:23:GLY:H     | 8:CI:60:LEU:HA     | 1.73                     | 0.54              |
| 10:CK:121:ARG:HE  | 21:CU:34:ARG:CG    | 2.21                     | 0.54              |
| 11:CL:88:ASP:C    | 11:CL:89:LEU:HD22  | 2.32                     | 0.54              |
| 12:CM:53:ASP:HA   | 12:CM:56:ARG:NH2   | 2.22                     | 0.54              |
| 19:CT:79:THR:HA   | 19:CT:82:ILE:HG12  | 1.90                     | 0.54              |
| 20:CB:46:VAL:CG1  | 20:CB:47:PRO:HD3   | 2.22                     | 0.54              |
| 20:CB:78:ALA:CB   | 20:CB:213:LEU:HD13 | 2.38                     | 0.54              |
| 23:DB:345:A:H1'   | 23:DB:346:A:C2     | 2.41                     | 0.54              |
| 23:DB:1745:A:H2'  | 23:DB:1746:A:H8    | 1.73                     | 0.54              |
| 23:DB:2024:G:H5'' | 26:DD:154:LYS:HZ3  | 1.73                     | 0.54              |
| 23:DB:2323:G:C2'  | 23:DB:2324:U:H5'   | 2.37                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:DC:182:LYS:HE2  | 25:DC:264:LYS:NZ  | 2.23                     | 0.54              |
| 26:DD:56:LYS:HB3   | 26:DD:56:LYS:HZ2  | 1.72                     | 0.54              |
| 30:DH:86:ASP:C     | 30:DH:88:GLY:H    | 2.16                     | 0.54              |
| 31:DJ:93:ILE:CG2   | 31:DJ:97:PRO:HA   | 2.37                     | 0.54              |
| 33:DL:59:ARG:HA    | 50:D3:11:LYS:NZ   | 2.22                     | 0.54              |
| 34:DM:50:ARG:HA    | 34:DM:53:MET:HE2  | 1.90                     | 0.54              |
| 35:DN:8:ARG:HD3    | 35:DN:43:GLU:OE2  | 2.07                     | 0.54              |
| 35:DN:123:GLU:HG2  | 35:DN:124:ALA:H   | 1.72                     | 0.54              |
| 36:DO:35:ILE:HG21  | 36:DO:71:ALA:HA   | 1.90                     | 0.54              |
| 39:DR:80:ARG:HD2   | 39:DR:85:LYS:HA   | 1.90                     | 0.54              |
| 42:DU:9:GLU:OE1    | 42:DU:71:ILE:HG13 | 2.08                     | 0.54              |
| 42:DU:43:LYS:HZ2   | 42:DU:43:LYS:HB2  | 1.73                     | 0.54              |
| 43:DW:67:LYS:HG2   | 43:DW:71:LYS:CA   | 2.38                     | 0.54              |
| 48:D1:22:THR:HB    | 50:D3:34:LYS:HE3  | 1.90                     | 0.54              |
| 52:DI:41:PHE:CE2   | 52:DI:45:THR:HG21 | 2.43                     | 0.54              |
| 1:AA:916:U:H2'     | 1:AA:917:G:H8     | 1.72                     | 0.53              |
| 7:AH:76:ARG:HG2    | 7:AH:77:VAL:N     | 2.23                     | 0.53              |
| 20:AB:67:LEU:HD12  | 20:AB:153:MET:CE  | 2.38                     | 0.53              |
| 23:BB:636:G:O6     | 33:BL:76:GLU:HG2  | 2.08                     | 0.53              |
| 23:BB:1488:C:O2'   | 23:BB:1489:C:H5'  | 2.08                     | 0.53              |
| 23:BB:2199:A:H5'   | 23:BB:2200:C:OP2  | 2.07                     | 0.53              |
| 23:BB:2292:U:H2'   | 23:BB:2293:G:C8   | 2.44                     | 0.53              |
| 23:BB:2750:A:H5''  | 29:BG:3:VAL:HG13  | 1.90                     | 0.53              |
| 37:BP:8:GLU:HA     | 37:BP:11:GLN:CG   | 2.37                     | 0.53              |
| 37:BP:112:ARG:HH11 | 37:BP:112:ARG:HA  | 1.73                     | 0.53              |
| 41:BT:68:LYS:HD3   | 41:BT:68:LYS:O    | 2.08                     | 0.53              |
| 41:BT:69:ARG:H     | 41:BT:75:GLY:HA3  | 1.72                     | 0.53              |
| 52:BI:63:ASP:C     | 52:BI:65:SER:H    | 2.15                     | 0.53              |
| 1:CA:930:C:H2'     | 1:CA:931:C:H6     | 1.73                     | 0.53              |
| 1:CA:1245:C:H2'    | 1:CA:1246:A:H8    | 1.73                     | 0.53              |
| 2:CC:113:LYS:HA    | 2:CC:184:ASN:ND2  | 2.22                     | 0.53              |
| 3:CD:144:ILE:HD12  | 3:CD:154:VAL:HG11 | 1.89                     | 0.53              |
| 5:CF:51:ILE:HD13   | 5:CF:86:ARG:HG3   | 1.90                     | 0.53              |
| 16:CQ:17:GLU:C     | 16:CQ:19:SER:H    | 2.15                     | 0.53              |
| 19:CT:27:MET:O     | 19:CT:31:ILE:HG13 | 2.07                     | 0.53              |
| 19:CT:53:MET:HE3   | 19:CT:54:GLN:CA   | 2.36                     | 0.53              |
| 20:CB:40:ILE:CG2   | 20:CB:200:PRO:HB2 | 2.38                     | 0.53              |
| 20:CB:57:ASN:HB2   | 20:CB:219:THR:O   | 2.08                     | 0.53              |
| 22:DA:13:G:H4'     | 22:DA:15:A:H2'    | 1.89                     | 0.53              |
| 23:DB:873:C:H2'    | 23:DB:874:G:C8    | 2.43                     | 0.53              |
| 23:DB:1098:A:O2'   | 52:DI:4:VAL:C     | 2.50                     | 0.53              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:1413:A:H2'  | 23:DB:1414:C:C6    | 2.42                     | 0.53              |
| 23:DB:1549:A:H2'  | 23:DB:1550:C:C6    | 2.43                     | 0.53              |
| 23:DB:2216:G:H2'  | 23:DB:2217:G:C8    | 2.43                     | 0.53              |
| 23:DB:2743:U:C2'  | 23:DB:2744:G:H5''  | 2.38                     | 0.53              |
| 26:DD:5:VAL:HG22  | 26:DD:51:THR:O     | 2.08                     | 0.53              |
| 30:DH:121:VAL:O   | 30:DH:122:LEU:HB2  | 2.08                     | 0.53              |
| 34:DM:4:PRO:HD3   | 34:DM:47:GLU:CG    | 2.39                     | 0.53              |
| 34:DM:88:ASN:ND2  | 34:DM:88:ASN:N     | 2.56                     | 0.53              |
| 37:DP:29:VAL:CG2  | 37:DP:47:ILE:HD11  | 2.37                     | 0.53              |
| 39:DR:68:ARG:HB2  | 39:DR:97:LYS:HG3   | 1.90                     | 0.53              |
| 43:DW:9:THR:OG1   | 43:DW:10:ARG:N     | 2.40                     | 0.53              |
| 43:DW:75:ASN:C    | 43:DW:77:LYS:H     | 2.16                     | 0.53              |
| 46:DZ:3:LYS:HB2   | 46:DZ:7:PRO:HA     | 1.90                     | 0.53              |
| 47:D0:15:ARG:HH11 | 47:D0:15:ARG:HG3   | 1.73                     | 0.53              |
| 48:D1:35:LEU:HA   | 48:D1:48:TYR:O     | 2.08                     | 0.53              |
| 3:AD:1:ALA:O      | 3:AD:67:LEU:HD21   | 2.08                     | 0.53              |
| 3:AD:54:LEU:HD13  | 3:AD:54:LEU:C      | 2.33                     | 0.53              |
| 4:AE:158:LYS:HE2  | 4:AE:158:LYS:H     | 1.73                     | 0.53              |
| 6:AG:3:ARG:HB3    | 6:AG:3:ARG:CZ      | 2.37                     | 0.53              |
| 10:AK:61:ALA:O    | 10:AK:64:VAL:HG12  | 2.08                     | 0.53              |
| 10:AK:92:ARG:HB3  | 10:AK:92:ARG:NH1   | 2.20                     | 0.53              |
| 12:AM:44:ILE:HD12 | 12:AM:45:SER:N     | 2.20                     | 0.53              |
| 14:AO:60:SER:HA   | 14:AO:63:ARG:NH1   | 2.22                     | 0.53              |
| 17:AR:33:THR:HG23 | 17:AR:35:SER:H     | 1.72                     | 0.53              |
| 21:AU:29:ALA:HB1  | 21:AU:32:ARG:HH21  | 1.72                     | 0.53              |
| 23:BB:139:U:C5    | 41:BT:1:MET:HB2    | 2.44                     | 0.53              |
| 23:BB:418:C:H2'   | 23:BB:419:U:H6     | 1.73                     | 0.53              |
| 23:BB:1013:C:H2'  | 23:BB:1014:A:H8    | 1.73                     | 0.53              |
| 23:BB:1139:G:O2'  | 23:BB:1140:C:H5'   | 2.09                     | 0.53              |
| 23:BB:1259:G:H2'  | 23:BB:1260:A:C8    | 2.42                     | 0.53              |
| 23:BB:2204:G:H5'  | 25:BC:149:LYS:CE   | 2.25                     | 0.53              |
| 25:BC:28:PRO:HD2  | 25:BC:79:ARG:CZ    | 2.37                     | 0.53              |
| 27:BE:91:ASP:O    | 27:BE:92:HIS:HB2   | 2.06                     | 0.53              |
| 28:BF:3:LEU:O     | 28:BF:3:LEU:HD23   | 2.08                     | 0.53              |
| 32:BK:36:GLY:HA2  | 32:BK:62:VAL:O     | 2.09                     | 0.53              |
| 34:BM:67:VAL:CG2  | 34:BM:95:LEU:HD21  | 2.39                     | 0.53              |
| 35:BN:9:GLN:HE21  | 35:BN:17:ARG:NH1   | 2.07                     | 0.53              |
| 35:BN:52:ILE:HG21 | 35:BN:94:TYR:CD2   | 2.43                     | 0.53              |
| 35:BN:76:VAL:O    | 35:BN:79:LEU:HB2   | 2.08                     | 0.53              |
| 40:BS:29:VAL:CG1  | 40:BS:69:LEU:HB2   | 2.38                     | 0.53              |
| 40:BS:71:VAL:CG2  | 40:BS:107:VAL:HG12 | 2.30                     | 0.53              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:B3:11:LYS:HG2   | 50:B3:12:ARG:HG3   | 1.90                     | 0.53              |
| 1:CA:961:U:O4'     | 1:CA:961:U:O2      | 2.26                     | 0.53              |
| 1:CA:1001:C:H2'    | 1:CA:1002:G:H8     | 1.74                     | 0.53              |
| 1:CA:1347:G:N2     | 1:CA:1373:G:H2'    | 2.24                     | 0.53              |
| 1:CA:1468:A:O2'    | 1:CA:1469:C:H5'    | 2.08                     | 0.53              |
| 3:CD:22:SER:H      | 3:CD:109:THR:HG22  | 1.72                     | 0.53              |
| 3:CD:95:GLY:HA3    | 3:CD:135:GLN:NE2   | 2.24                     | 0.53              |
| 8:CI:62:LEU:N      | 8:CI:62:LEU:HD13   | 2.23                     | 0.53              |
| 15:CP:67:ILE:HG12  | 15:CP:72:ALA:HB2   | 1.91                     | 0.53              |
| 22:DA:32:U:H4'     | 22:DA:52:A:N6      | 2.23                     | 0.53              |
| 23:DB:27:G:N2      | 23:DB:512:G:H2'    | 2.16                     | 0.53              |
| 23:DB:65:U:H2'     | 23:DB:66:C:C6      | 2.42                     | 0.53              |
| 23:DB:251:A:H2'    | 23:DB:252:G:O4'    | 2.08                     | 0.53              |
| 23:DB:2186:G:O2'   | 23:DB:2187:U:H5'   | 2.07                     | 0.53              |
| 23:DB:2311:A:N3    | 28:DF:39:VAL:HB    | 2.22                     | 0.53              |
| 25:DC:153:LEU:C    | 25:DC:155:ARG:H    | 2.17                     | 0.53              |
| 26:DD:17:GLU:OE2   | 32:DK:72:PRO:HB2   | 2.08                     | 0.53              |
| 28:DF:137:PHE:O    | 28:DF:139:GLU:N    | 2.41                     | 0.53              |
| 30:DH:122:LEU:HD13 | 30:DH:146:VAL:HG13 | 1.90                     | 0.53              |
| 31:DJ:100:VAL:HG22 | 31:DJ:101:ILE:H    | 1.72                     | 0.53              |
| 33:DL:58:TYR:HB3   | 50:D3:13:PHE:CE1   | 2.42                     | 0.53              |
| 37:DP:90:ALA:HB3   | 37:DP:111:GLU:CB   | 2.38                     | 0.53              |
| 39:DR:69:GLY:CA    | 39:DR:96:VAL:HG13  | 2.39                     | 0.53              |
| 46:DZ:24:ILE:H     | 46:DZ:24:ILE:CD1   | 2.14                     | 0.53              |
| 1:AA:203:G:N2      | 1:AA:205:A:N6      | 2.57                     | 0.53              |
| 1:AA:474:G:H2'     | 1:AA:475:C:H6      | 1.73                     | 0.53              |
| 1:AA:730:G:O2'     | 1:AA:766:A:H5'     | 2.08                     | 0.53              |
| 1:AA:1130:A:H5'    | 8:AI:19:PHE:CE2    | 2.43                     | 0.53              |
| 1:AA:1237:C:H4'    | 1:AA:1334:G:N2     | 2.24                     | 0.53              |
| 2:AC:110:LEU:O     | 2:AC:203:LYS:HE2   | 2.08                     | 0.53              |
| 8:AI:71:ILE:H      | 8:AI:71:ILE:CD1    | 2.20                     | 0.53              |
| 9:AJ:67:ILE:HG12   | 13:AN:94:GLY:O     | 2.08                     | 0.53              |
| 15:AP:40:ASN:HD21  | 15:AP:42:ILE:HG13  | 1.73                     | 0.53              |
| 20:AB:79:VAL:HG11  | 20:AB:92:ASN:HB3   | 1.89                     | 0.53              |
| 23:BB:152:A:H2'    | 23:BB:153:U:C6     | 2.43                     | 0.53              |
| 23:BB:155:A:H2'    | 23:BB:156:A:H8     | 1.68                     | 0.53              |
| 23:BB:696:G:O2'    | 23:BB:697:G:H5'    | 2.07                     | 0.53              |
| 23:BB:711:G:O2'    | 23:BB:712:G:H5'    | 2.09                     | 0.53              |
| 23:BB:877:A:H2'    | 23:BB:899:A:N1     | 2.24                     | 0.53              |
| 23:BB:1204:A:N1    | 23:BB:1241:A:N1    | 2.55                     | 0.53              |
| 23:BB:1231:U:H2'   | 23:BB:1232:G:H8    | 1.73                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BB:1629:U:O2   | 23:BB:2698:U:H5'' | 2.08                     | 0.53              |
| 23:BB:2053:G:C2'  | 23:BB:2054:A:H5'  | 2.37                     | 0.53              |
| 23:BB:2774:C:H2'  | 23:BB:2775:G:O4'  | 2.09                     | 0.53              |
| 23:BB:2848:G:H1'  | 23:BB:2868:A:H61  | 1.72                     | 0.53              |
| 24:BV:84:PRO:HG3  | 34:BM:127:LYS:CE  | 2.37                     | 0.53              |
| 26:BD:59:ARG:HH21 | 26:BD:60:VAL:CG1  | 2.22                     | 0.53              |
| 26:BD:59:ARG:HH21 | 26:BD:60:VAL:HG12 | 1.73                     | 0.53              |
| 26:BD:62:LYS:N    | 26:BD:63:PRO:HD2  | 2.23                     | 0.53              |
| 29:BG:17:LYS:HE3  | 29:BG:24:THR:CG2  | 2.37                     | 0.53              |
| 30:BH:1:MET:HB2   | 30:BH:20:ASN:OD1  | 2.09                     | 0.53              |
| 31:BJ:72:LYS:HB3  | 31:BJ:74:TYR:CE2  | 2.43                     | 0.53              |
| 34:BM:73:ILE:HG22 | 34:BM:74:THR:N    | 2.24                     | 0.53              |
| 37:BP:69:VAL:O    | 37:BP:70:GLU:HB2  | 2.09                     | 0.53              |
| 46:BZ:25:ARG:HG3  | 46:BZ:26:SER:N    | 2.24                     | 0.53              |
| 52:BI:23:VAL:HG23 | 52:BI:24:GLY:N    | 2.24                     | 0.53              |
| 52:BI:37:PHE:HB2  | 52:BI:66:PHE:CZ   | 2.44                     | 0.53              |
| 1:CA:317:U:H2'    | 1:CA:318:G:H8     | 1.73                     | 0.53              |
| 1:CA:545:C:H5''   | 3:CD:68:GLU:HG2   | 1.90                     | 0.53              |
| 1:CA:672:U:H2'    | 1:CA:673:A:C8     | 2.43                     | 0.53              |
| 1:CA:677:U:H2'    | 1:CA:678:U:C6     | 2.44                     | 0.53              |
| 1:CA:860:A:H2'    | 1:CA:861:G:O4'    | 2.09                     | 0.53              |
| 1:CA:1252:A:H2'   | 1:CA:1253:G:O4'   | 2.08                     | 0.53              |
| 2:CC:116:ALA:HB1  | 2:CC:186:SER:OG   | 2.07                     | 0.53              |
| 5:CF:10:VAL:HG12  | 5:CF:11:HIS:N     | 2.23                     | 0.53              |
| 6:CG:14:ASP:HB3   | 6:CG:18:GLY:H     | 1.73                     | 0.53              |
| 9:CJ:82:LYS:N     | 9:CJ:82:LYS:HD2   | 2.23                     | 0.53              |
| 14:CO:83:ARG:C    | 14:CO:84:LEU:HD12 | 2.33                     | 0.53              |
| 18:CS:15:LEU:O    | 18:CS:15:LEU:HD23 | 2.08                     | 0.53              |
| 23:DB:6:A:H4'     | 31:DJ:133:ALA:O   | 2.08                     | 0.53              |
| 23:DB:905:A:O2'   | 23:DB:906:U:H5'   | 2.09                     | 0.53              |
| 23:DB:1080:A:O2'  | 52:DI:126:ARG:HD2 | 2.08                     | 0.53              |
| 23:DB:1100:C:H2'  | 23:DB:1101:U:C6   | 2.44                     | 0.53              |
| 23:DB:1172:C:H2'  | 23:DB:1173:U:O4'  | 2.07                     | 0.53              |
| 23:DB:1682:G:C2   | 23:DB:1757:A:O4'  | 2.61                     | 0.53              |
| 23:DB:1716:U:H2'  | 23:DB:1717:A:C8   | 2.43                     | 0.53              |
| 23:DB:2077:A:O2'  | 23:DB:2078:C:H5'  | 2.08                     | 0.53              |
| 25:DC:22:GLU:HB2  | 25:DC:202:ARG:CG  | 2.38                     | 0.53              |
| 25:DC:137:GLY:C   | 25:DC:139:THR:N   | 2.66                     | 0.53              |
| 25:DC:245:THR:O   | 25:DC:247:TRP:N   | 2.40                     | 0.53              |
| 27:DE:154:ASP:CG  | 27:DE:156:ASN:H   | 2.17                     | 0.53              |
| 28:DF:100:GLU:C   | 28:DF:102:LEU:H   | 2.15                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:DG:25:ILE:HD11 | 29:DG:75:VAL:HG22  | 1.89                     | 0.53              |
| 31:DJ:131:ASN:C   | 31:DJ:133:ALA:N    | 2.64                     | 0.53              |
| 32:DK:43:ILE:HD11 | 32:DK:58:LEU:HD21  | 1.90                     | 0.53              |
| 33:DL:96:LYS:HE3  | 33:DL:96:LYS:CA    | 2.38                     | 0.53              |
| 40:DS:74:ILE:CG2  | 40:DS:105:VAL:HG23 | 2.38                     | 0.53              |
| 1:AA:128:G:H2'    | 1:AA:129:A:C8      | 2.43                     | 0.53              |
| 1:AA:817:C:H1'    | 1:AA:819:A:C5'     | 2.38                     | 0.53              |
| 1:AA:982:U:H4'    | 1:AA:983:A:O4'     | 2.08                     | 0.53              |
| 1:AA:1314:C:H2'   | 1:AA:1315:U:C6     | 2.44                     | 0.53              |
| 7:AH:42:GLU:HG3   | 7:AH:100:ILE:HD13  | 1.90                     | 0.53              |
| 8:AI:30:ASN:N     | 8:AI:30:ASN:HD22   | 2.06                     | 0.53              |
| 12:AM:52:ILE:HD12 | 12:AM:55:LEU:HD12  | 1.90                     | 0.53              |
| 14:AO:11:VAL:HA   | 14:AO:26:VAL:HG13  | 1.90                     | 0.53              |
| 14:AO:24:THR:HB   | 14:AO:69:LEU:HD21  | 1.90                     | 0.53              |
| 14:AO:80:LEU:HD23 | 14:AO:80:LEU:C     | 2.33                     | 0.53              |
| 18:AS:12:LEU:HG   | 18:AS:15:LEU:HD23  | 1.91                     | 0.53              |
| 22:BA:35:C:H2'    | 22:BA:36:C:O4'     | 2.08                     | 0.53              |
| 23:BB:852:U:H2'   | 23:BB:853:C:H6     | 1.72                     | 0.53              |
| 23:BB:987:C:H2'   | 23:BB:988:A:O4'    | 2.08                     | 0.53              |
| 23:BB:992:C:H2'   | 23:BB:993:G:H8     | 1.74                     | 0.53              |
| 23:BB:1159:U:H2'  | 23:BB:1160:G:C8    | 2.43                     | 0.53              |
| 23:BB:1387:A:H2'  | 23:BB:1388:G:C8    | 2.41                     | 0.53              |
| 23:BB:1439:A:N6   | 23:BB:1440:U:O2    | 2.35                     | 0.53              |
| 23:BB:1487:U:H2'  | 23:BB:1488:C:H6    | 1.73                     | 0.53              |
| 23:BB:1571:A:H2'  | 23:BB:1572:A:H8    | 1.73                     | 0.53              |
| 23:BB:1733:G:H2'  | 23:BB:1734:G:H8    | 1.74                     | 0.53              |
| 23:BB:1842:G:H2'  | 23:BB:1843:C:C6    | 2.44                     | 0.53              |
| 23:BB:2305:U:H1'  | 28:BF:132:ARG:HA   | 1.90                     | 0.53              |
| 23:BB:2405:G:H1'  | 23:BB:2412:A:N6    | 2.23                     | 0.53              |
| 23:BB:2636:C:H4'  | 26:BD:80:TRP:CE3   | 2.43                     | 0.53              |
| 23:BB:2772:C:H5'' | 26:BD:171:THR:HG21 | 1.91                     | 0.53              |
| 24:BV:57:TYR:CD2  | 34:BM:133:LYS:HE2  | 2.43                     | 0.53              |
| 25:BC:155:ARG:NE  | 25:BC:157:ALA:HB3  | 2.16                     | 0.53              |
| 25:BC:222:THR:C   | 25:BC:224:MET:H    | 2.16                     | 0.53              |
| 29:BG:78:VAL:HG23 | 29:BG:79:THR:HG23  | 1.91                     | 0.53              |
| 29:BG:169:ARG:C   | 29:BG:171:LYS:H    | 2.17                     | 0.53              |
| 30:BH:9:VAL:C     | 30:BH:11:ASN:H     | 2.17                     | 0.53              |
| 31:BJ:43:GLU:O    | 31:BJ:45:THR:N     | 2.42                     | 0.53              |
| 31:BJ:84:ILE:HG22 | 31:BJ:85:LYS:H     | 1.73                     | 0.53              |
| 33:BL:38:GLN:C    | 33:BL:40:SER:N     | 2.65                     | 0.53              |
| 33:BL:64:PHE:H    | 50:B3:24:LYS:CD    | 2.14                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:BM:95:LEU:HD22 | 34:BM:98:PRO:CG    | 2.36                     | 0.53              |
| 37:BP:108:ARG:H   | 37:BP:108:ARG:CD   | 2.21                     | 0.53              |
| 38:BQ:27:ARG:HA   | 38:BQ:33:VAL:HB    | 1.90                     | 0.53              |
| 39:BR:62:GLU:HG3  | 39:BR:103:ALA:HA   | 1.89                     | 0.53              |
| 50:B3:4:LYS:HZ1   | 50:B3:59:ALA:H     | 1.56                     | 0.53              |
| 1:CA:787:A:O2'    | 1:CA:788:U:H5'     | 2.08                     | 0.53              |
| 1:CA:1412:C:H2'   | 1:CA:1413:A:H8     | 1.72                     | 0.53              |
| 4:CE:104:ILE:HG13 | 4:CE:114:LEU:HB2   | 1.89                     | 0.53              |
| 8:CI:24:ASN:OD1   | 8:CI:26:LYS:HG2    | 2.09                     | 0.53              |
| 12:CM:95:PRO:HD3  | 12:CM:108:ARG:HG2  | 1.88                     | 0.53              |
| 20:CB:62:ARG:H    | 20:CB:62:ARG:CD    | 2.22                     | 0.53              |
| 20:CB:86:CYS:HB3  | 20:CB:88:GLN:NE2   | 2.22                     | 0.53              |
| 22:DA:21:G:H2'    | 22:DA:22:U:O4'     | 2.08                     | 0.53              |
| 22:DA:53:A:O2'    | 22:DA:54:G:H5'     | 2.07                     | 0.53              |
| 23:DB:130:C:O2'   | 23:DB:131:A:H5'    | 2.08                     | 0.53              |
| 23:DB:247:G:H4'   | 23:DB:386:G:C4     | 2.43                     | 0.53              |
| 23:DB:545:U:H3'   | 23:DB:546:U:H5''   | 1.91                     | 0.53              |
| 23:DB:1051:G:H2'  | 23:DB:1052:C:H6    | 1.73                     | 0.53              |
| 23:DB:1198:U:C2   | 23:DB:1199:U:C5    | 2.97                     | 0.53              |
| 23:DB:1751:U:H2'  | 23:DB:1752:C:C6    | 2.43                     | 0.53              |
| 23:DB:2247:A:H2'  | 23:DB:2248:C:H6    | 1.71                     | 0.53              |
| 23:DB:2874:C:H2'  | 23:DB:2875:C:C6    | 2.42                     | 0.53              |
| 26:DD:79:LEU:CG   | 26:DD:80:TRP:H     | 2.20                     | 0.53              |
| 27:DE:191:ASP:HA  | 27:DE:194:LYS:CE   | 2.39                     | 0.53              |
| 28:DF:168:LEU:O   | 28:DF:168:LEU:HD23 | 2.09                     | 0.53              |
| 29:DG:39:ALA:HA   | 29:DG:54:ARG:HB2   | 1.90                     | 0.53              |
| 30:DH:90:LEU:HD22 | 30:DH:122:LEU:O    | 2.07                     | 0.53              |
| 30:DH:95:GLY:O    | 30:DH:99:ILE:HG12  | 2.08                     | 0.53              |
| 31:DJ:23:LYS:HE3  | 31:DJ:63:ALA:CB    | 2.38                     | 0.53              |
| 31:DJ:28:LEU:C    | 31:DJ:28:LEU:HD13  | 2.32                     | 0.53              |
| 34:DM:86:LYS:HG2  | 34:DM:87:GLY:H     | 1.73                     | 0.53              |
| 37:DP:32:VAL:HA   | 37:DP:42:PHE:CB    | 2.34                     | 0.53              |
| 41:DT:6:ARG:HG2   | 41:DT:9:LYS:O      | 2.09                     | 0.53              |
| 43:DW:30:VAL:HG12 | 43:DW:31:LEU:N     | 2.23                     | 0.53              |
| 45:DY:1:ALA:N     | 45:DY:43:ILE:HB    | 2.23                     | 0.53              |
| 51:D4:2:LYS:HG2   | 51:D4:38:GLY:HA3   | 1.90                     | 0.53              |
| 51:D4:23:ILE:HD12 | 51:D4:24:ARG:HD2   | 1.90                     | 0.53              |
| 52:DI:92:PRO:O    | 52:DI:93:ASN:HB2   | 2.07                     | 0.53              |
| 52:DI:102:ARG:HG3 | 52:DI:141:ASP:CB   | 2.38                     | 0.53              |
| 1:AA:610:U:O4'    | 1:AA:610:U:O2      | 2.25                     | 0.53              |
| 1:AA:845:A:H3'    | 1:AA:846:G:O4'     | 2.08                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 20:AB:165:ALA:CB  | 20:AB:186:VAL:HG12 | 2.38                     | 0.53              |
| 23:BB:254:G:O6    | 50:B3:3:ILE:HG23   | 2.09                     | 0.53              |
| 23:BB:520:G:H2'   | 23:BB:521:U:C6     | 2.43                     | 0.53              |
| 23:BB:716:A:H3'   | 23:BB:717:C:H5''   | 1.90                     | 0.53              |
| 23:BB:1220:G:H2'  | 23:BB:1221:C:H6    | 1.72                     | 0.53              |
| 23:BB:2304:G:H22  | 23:BB:2312:U:H3    | 1.56                     | 0.53              |
| 23:BB:2794:C:H2'  | 23:BB:2795:C:C6    | 2.44                     | 0.53              |
| 24:BV:82:TYR:N    | 24:BV:82:TYR:CD2   | 2.76                     | 0.53              |
| 27:BE:44:ARG:H    | 27:BE:44:ARG:CD    | 2.21                     | 0.53              |
| 29:BG:26:LYS:HG2  | 29:BG:31:GLU:HG2   | 1.90                     | 0.53              |
| 29:BG:90:GLY:HA3  | 29:BG:93:TYR:CD2   | 2.44                     | 0.53              |
| 34:BM:67:VAL:HG23 | 34:BM:95:LEU:HD21  | 1.89                     | 0.53              |
| 40:BS:69:LEU:N    | 40:BS:69:LEU:HD22  | 2.24                     | 0.53              |
| 1:CA:633:G:H2'    | 1:CA:634:C:C6      | 2.44                     | 0.53              |
| 1:CA:920:U:H2'    | 1:CA:921:U:C6      | 2.43                     | 0.53              |
| 5:CF:51:ILE:CD1   | 5:CF:86:ARG:HG3    | 2.39                     | 0.53              |
| 17:CR:62:ARG:C    | 17:CR:64:LEU:H     | 2.15                     | 0.53              |
| 23:DB:1545:A:H2'  | 23:DB:1546:G:O4'   | 2.09                     | 0.53              |
| 23:DB:1813:G:H1'  | 25:DC:45:ASN:HB3   | 1.90                     | 0.53              |
| 23:DB:1842:G:H2'  | 23:DB:1843:C:C6    | 2.43                     | 0.53              |
| 23:DB:2723:C:H5'  | 35:DN:4:ARG:NH2    | 2.24                     | 0.53              |
| 25:DC:28:PRO:O    | 25:DC:29:PHE:CG    | 2.61                     | 0.53              |
| 25:DC:53:ILE:CG1  | 25:DC:218:THR:HA   | 2.37                     | 0.53              |
| 25:DC:145:MET:HE1 | 25:DC:181:ARG:NH2  | 2.23                     | 0.53              |
| 26:DD:124:ARG:NH1 | 26:DD:160:LYS:HE2  | 2.24                     | 0.53              |
| 26:DD:173:GLN:HG2 | 26:DD:208:LYS:HB3  | 1.90                     | 0.53              |
| 29:DG:169:ARG:HB2 | 29:DG:169:ARG:CZ   | 2.37                     | 0.53              |
| 32:DK:38:ILE:HD13 | 32:DK:61:VAL:HG12  | 1.91                     | 0.53              |
| 32:DK:70:ARG:O    | 32:DK:71:ARG:HG2   | 2.08                     | 0.53              |
| 32:DK:93:GLN:CG   | 32:DK:94:PRO:HD2   | 2.38                     | 0.53              |
| 33:DL:79:LEU:CD1  | 33:DL:112:LEU:HD23 | 2.39                     | 0.53              |
| 35:DN:24:MET:HG2  | 35:DN:44:LEU:HD13  | 1.91                     | 0.53              |
| 35:DN:42:LYS:CE   | 35:DN:45:ARG:HG3   | 2.37                     | 0.53              |
| 40:DS:84:ARG:HH21 | 40:DS:98:LYS:HZ3   | 1.56                     | 0.53              |
| 41:DT:31:VAL:HG22 | 41:DT:32:LEU:N     | 2.24                     | 0.53              |
| 45:DY:4:ILE:HG23  | 45:DY:5:LYS:HD3    | 1.91                     | 0.53              |
| 1:AA:600:A:H2'    | 1:AA:601:G:H8      | 1.73                     | 0.53              |
| 1:AA:633:G:H2'    | 1:AA:634:C:C6      | 2.44                     | 0.53              |
| 1:AA:1027:C:H2'   | 1:AA:1028:C:C6     | 2.43                     | 0.53              |
| 2:AC:40:GLN:O     | 2:AC:44:LYS:HG3    | 2.08                     | 0.53              |
| 2:AC:85:LYS:O     | 2:AC:89:VAL:HG23   | 2.08                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:AG:129:ASN:HA   | 6:AG:134:VAL:HG21 | 1.89                     | 0.53              |
| 13:AN:59:GLN:NE2  | 13:AN:59:GLN:N    | 2.56                     | 0.53              |
| 18:AS:10:ILE:HG22 | 18:AS:38:THR:H    | 1.73                     | 0.53              |
| 23:BB:298:G:OP1   | 42:BU:82:VAL:HA   | 2.09                     | 0.53              |
| 23:BB:460:A:H2'   | 23:BB:461:C:O4'   | 2.09                     | 0.53              |
| 23:BB:710:U:H2'   | 23:BB:711:G:C8    | 2.42                     | 0.53              |
| 23:BB:817:C:O2'   | 23:BB:839:U:H5''  | 2.09                     | 0.53              |
| 23:BB:910:A:H2    | 23:BB:2264:C:O2   | 1.92                     | 0.53              |
| 23:BB:948:C:H2'   | 23:BB:949:G:H8    | 1.74                     | 0.53              |
| 23:BB:1006:C:O2'  | 23:BB:1007:C:H5'  | 2.08                     | 0.53              |
| 23:BB:1028:A:N6   | 23:BB:1125:G:H2'  | 2.24                     | 0.53              |
| 23:BB:1131:G:C4'  | 31:BJ:85:LYS:HZ2  | 2.22                     | 0.53              |
| 23:BB:1684:G:H2'  | 23:BB:1685:C:C6   | 2.44                     | 0.53              |
| 23:BB:2097:A:H2'  | 23:BB:2098:U:H6   | 1.73                     | 0.53              |
| 23:BB:2692:G:O2'  | 23:BB:2693:G:H5'  | 2.08                     | 0.53              |
| 23:BB:2874:C:H2'  | 23:BB:2875:C:C6   | 2.43                     | 0.53              |
| 23:BB:2899:A:H2'  | 23:BB:2900:A:H8   | 1.74                     | 0.53              |
| 25:BC:58:LYS:HB2  | 25:BC:58:LYS:NZ   | 2.24                     | 0.53              |
| 31:BJ:10:THR:HB   | 31:BJ:13:ARG:NH1  | 2.24                     | 0.53              |
| 34:BM:108:VAL:O   | 34:BM:110:GLU:N   | 2.42                     | 0.53              |
| 39:BR:5:PHE:CE2   | 39:BR:7:SER:HB3   | 2.44                     | 0.53              |
| 43:BW:76:ARG:CZ   | 43:BW:76:ARG:HB3  | 2.38                     | 0.53              |
| 1:CA:140:U:H2'    | 1:CA:141:G:H8     | 1.73                     | 0.53              |
| 1:CA:149:A:H1'    | 1:CA:1446:A:C2    | 2.44                     | 0.53              |
| 1:CA:437:U:C2'    | 1:CA:438:U:O4'    | 2.51                     | 0.53              |
| 1:CA:471:U:H2'    | 1:CA:472:U:H6     | 1.73                     | 0.53              |
| 1:CA:521:G:OP1    | 11:CL:69:GLU:HB3  | 2.08                     | 0.53              |
| 1:CA:613:C:H2'    | 1:CA:614:C:C6     | 2.44                     | 0.53              |
| 1:CA:736:C:H2'    | 1:CA:737:C:C6     | 2.43                     | 0.53              |
| 1:CA:1026:G:H2'   | 1:CA:1027:C:C6    | 2.41                     | 0.53              |
| 1:CA:1060:U:H2'   | 1:CA:1061:G:C8    | 2.44                     | 0.53              |
| 1:CA:1283:U:O2'   | 1:CA:1284:C:H5'   | 2.08                     | 0.53              |
| 4:CE:35:LEU:HD13  | 4:CE:133:ILE:HA   | 1.91                     | 0.53              |
| 4:CE:110:MET:HG2  | 4:CE:139:THR:OG1  | 2.09                     | 0.53              |
| 8:CI:51:LEU:HD22  | 8:CI:56:MET:HG2   | 1.90                     | 0.53              |
| 9:CJ:51:VAL:CG2   | 13:CN:80:ARG:HB2  | 2.33                     | 0.53              |
| 20:CB:102:ASN:ND2 | 20:CB:105:THR:HB  | 2.24                     | 0.53              |
| 22:DA:94:A:O2'    | 22:DA:95:U:H5'    | 2.08                     | 0.53              |
| 23:DB:417:C:H2'   | 23:DB:418:C:C6    | 2.44                     | 0.53              |
| 23:DB:635:C:P     | 33:DL:126:ARG:HE  | 2.32                     | 0.53              |
| 23:DB:945:A:H3'   | 23:DB:946:C:H5''  | 1.90                     | 0.53              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:1082:U:C4    | 23:DB:1086:A:N1    | 2.77                     | 0.53              |
| 23:DB:1791:A:C5'   | 25:DC:211:ARG:HE   | 2.20                     | 0.53              |
| 23:DB:1813:G:N3    | 25:DC:50:THR:CG2   | 2.69                     | 0.53              |
| 23:DB:1946:U:H2'   | 23:DB:1947:C:C6    | 2.43                     | 0.53              |
| 23:DB:2641:G:OP1   | 31:DJ:78:THR:HG22  | 2.09                     | 0.53              |
| 23:DB:2820:A:N6    | 26:DD:197:THR:HB   | 2.24                     | 0.53              |
| 25:DC:28:PRO:HD2   | 25:DC:79:ARG:HE    | 1.73                     | 0.53              |
| 25:DC:152:GLN:HB3  | 25:DC:153:LEU:HD23 | 1.90                     | 0.53              |
| 29:DG:11:PRO:HD2   | 29:DG:14:VAL:HG21  | 1.90                     | 0.53              |
| 32:DK:108:ARG:HH11 | 32:DK:108:ARG:HG3  | 1.73                     | 0.53              |
| 33:DL:115:GLU:C    | 33:DL:116:VAL:HG13 | 2.34                     | 0.53              |
| 36:DO:30:ARG:HD2   | 36:DO:97:PHE:HD2   | 1.74                     | 0.53              |
| 37:DP:31:VAL:HG12  | 37:DP:33:GLU:H     | 1.72                     | 0.53              |
| 39:DR:4:VAL:HG12   | 39:DR:43:ASN:CB    | 2.38                     | 0.53              |
| 39:DR:44:GLY:N     | 39:DR:53:PHE:HE2   | 2.06                     | 0.53              |
| 40:DS:27:LYS:HA    | 40:DS:70:LYS:CB    | 2.38                     | 0.53              |
| 41:DT:7:LEU:H      | 41:DT:7:LEU:HD22   | 1.73                     | 0.53              |
| 43:DW:21:GLY:HA2   | 43:DW:25:PHE:CE1   | 2.43                     | 0.53              |
| 44:DX:17:GLU:O     | 44:DX:22:LEU:HG    | 2.08                     | 0.53              |
| 48:D1:8:ILE:CD1    | 48:D1:9:LYS:H      | 2.22                     | 0.53              |
| 52:DI:1:ALA:HB1    | 52:DI:2:LYS:HD2    | 1.90                     | 0.53              |
| 52:DI:54:ILE:HD13  | 52:DI:55:PRO:N     | 2.22                     | 0.53              |
| 1:AA:113:G:H2'     | 1:AA:114:U:C6      | 2.43                     | 0.53              |
| 1:AA:252:U:H2'     | 1:AA:253:A:H8      | 1.74                     | 0.53              |
| 1:AA:287:U:O2'     | 1:AA:288:A:H5'     | 2.08                     | 0.53              |
| 2:AC:139:ASN:O     | 2:AC:143:LEU:HD22  | 2.09                     | 0.53              |
| 9:AJ:35:GLN:H      | 9:AJ:78:GLU:HB3    | 1.74                     | 0.53              |
| 11:AL:79:ILE:HG22  | 11:AL:103:CYS:HB2  | 1.90                     | 0.53              |
| 11:AL:80:LEU:HD23  | 11:AL:97:VAL:HG21  | 1.90                     | 0.53              |
| 13:AN:61:ASN:O     | 13:AN:62:ARG:HB2   | 2.07                     | 0.53              |
| 13:AN:82:LYS:HE2   | 13:AN:82:LYS:HA    | 1.91                     | 0.53              |
| 16:AQ:28:VAL:C     | 16:AQ:36:PHE:HA    | 2.33                     | 0.53              |
| 18:AS:10:ILE:HD13  | 18:AS:40:PHE:CE1   | 2.44                     | 0.53              |
| 18:AS:31:ARG:HH11  | 18:AS:31:ARG:HG2   | 1.74                     | 0.53              |
| 22:BA:17:C:C2'     | 22:BA:18:G:H5'     | 2.39                     | 0.53              |
| 23:BB:257:C:H2'    | 23:BB:258:G:O4'    | 2.09                     | 0.53              |
| 23:BB:309:A:N3     | 23:BB:329:G:O2'    | 2.42                     | 0.53              |
| 23:BB:560:C:H3'    | 23:BB:561:G:C8     | 2.44                     | 0.53              |
| 23:BB:664:G:H2'    | 23:BB:665:U:C6     | 2.44                     | 0.53              |
| 23:BB:847:U:O4'    | 23:BB:847:U:O2     | 2.27                     | 0.53              |
| 23:BB:1060:U:O2    | 23:BB:1088:A:C8    | 2.62                     | 0.53              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:1583:A:H4'   | 23:BB:1585:C:C4    | 2.44                     | 0.53              |
| 23:BB:1671:U:H2'   | 23:BB:1673:G:OP2   | 2.08                     | 0.53              |
| 23:BB:1864:U:O2'   | 23:BB:1865:U:H5'   | 2.08                     | 0.53              |
| 23:BB:2634:A:H2'   | 23:BB:2635:A:C8    | 2.44                     | 0.53              |
| 26:BD:60:VAL:HB    | 26:BD:63:PRO:CG    | 2.38                     | 0.53              |
| 26:BD:131:ASP:OD2  | 26:BD:133:THR:HG22 | 2.08                     | 0.53              |
| 27:BE:44:ARG:HD3   | 27:BE:44:ARG:N     | 2.24                     | 0.53              |
| 31:BJ:72:LYS:CB    | 31:BJ:90:GLU:HB2   | 2.34                     | 0.53              |
| 31:BJ:78:THR:O     | 31:BJ:80:HIS:N     | 2.42                     | 0.53              |
| 34:BM:82:MET:CB    | 34:BM:84:LYS:HZ2   | 2.14                     | 0.53              |
| 41:BT:6:ARG:C      | 41:BT:8:LEU:N      | 2.67                     | 0.53              |
| 43:BW:47:GLY:CA    | 43:BW:67:LYS:HZ3   | 2.21                     | 0.53              |
| 45:BY:4:ILE:HG12   | 45:BY:5:LYS:HE2    | 1.90                     | 0.53              |
| 46:BZ:5:ILE:HD13   | 46:BZ:51:VAL:HG12  | 1.91                     | 0.53              |
| 48:B1:42:VAL:CG1   | 48:B1:43:ARG:N     | 2.72                     | 0.53              |
| 1:CA:276:G:H5'     | 16:CQ:16:MET:SD    | 2.48                     | 0.53              |
| 1:CA:817:C:H1'     | 1:CA:819:A:C5'     | 2.38                     | 0.53              |
| 1:CA:952:U:H2'     | 1:CA:953:G:C8      | 2.41                     | 0.53              |
| 2:CC:49:ALA:HB2    | 2:CC:74:ILE:HG21   | 1.91                     | 0.53              |
| 2:CC:89:VAL:HG23   | 2:CC:90:VAL:N      | 2.23                     | 0.53              |
| 3:CD:104:MET:SD    | 3:CD:179:GLY:HA2   | 2.47                     | 0.53              |
| 4:CE:136:VAL:HG23  | 4:CE:137:ARG:N     | 2.23                     | 0.53              |
| 12:CM:15:VAL:HG13  | 12:CM:40:GLU:HB2   | 1.89                     | 0.53              |
| 15:CP:3:THR:HB     | 15:CP:66:THR:O     | 2.07                     | 0.53              |
| 20:CB:40:ILE:HG21  | 20:CB:200:PRO:O    | 2.09                     | 0.53              |
| 23:DB:633:A:C2'    | 23:DB:634:C:H5'    | 2.37                     | 0.53              |
| 23:DB:937:C:H2'    | 23:DB:938:G:C8     | 2.43                     | 0.53              |
| 23:DB:1341:G:H2'   | 23:DB:1397:U:O2'   | 2.09                     | 0.53              |
| 23:DB:1583:A:H4'   | 23:DB:1585:C:C4    | 2.44                     | 0.53              |
| 23:DB:1733:G:H2'   | 23:DB:1734:G:H8    | 1.73                     | 0.53              |
| 23:DB:1826:G:H2'   | 23:DB:1827:U:C6    | 2.44                     | 0.53              |
| 23:DB:2348:U:O2'   | 23:DB:2349:G:H5'   | 2.09                     | 0.53              |
| 23:DB:2718:G:O2'   | 23:DB:2719:G:H5'   | 2.09                     | 0.53              |
| 25:DC:123:ILE:HG12 | 25:DC:135:PRO:CD   | 2.39                     | 0.53              |
| 25:DC:168:GLY:C    | 25:DC:170:TYR:H    | 2.16                     | 0.53              |
| 25:DC:224:MET:O    | 25:DC:225:ASN:HB2  | 2.07                     | 0.53              |
| 27:DE:15:SER:O     | 27:DE:17:THR:HG22  | 2.09                     | 0.53              |
| 27:DE:161:ALA:O    | 27:DE:162:ARG:HB2  | 2.07                     | 0.53              |
| 31:DJ:40:HIS:O     | 38:DQ:66:ALA:HB1   | 2.09                     | 0.53              |
| 33:DL:58:TYR:HB3   | 50:D3:13:PHE:HZ    | 1.73                     | 0.53              |
| 35:DN:32:GLU:O     | 35:DN:114:GLU:HA   | 2.08                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:DO:25:ARG:O    | 36:DO:26:LEU:HD12  | 2.09                     | 0.53              |
| 38:DQ:40:LYS:HB2  | 38:DQ:40:LYS:NZ    | 2.23                     | 0.53              |
| 40:DS:31:GLN:O    | 40:DS:35:ILE:HG13  | 2.08                     | 0.53              |
| 43:DW:44:PHE:HB3  | 43:DW:77:LYS:C     | 2.34                     | 0.53              |
| 49:D2:6:GLN:HB3   | 49:D2:7:PRO:HD2    | 1.89                     | 0.53              |
| 1:AA:613:C:H2'    | 1:AA:614:C:C6      | 2.44                     | 0.53              |
| 1:AA:640:A:O2'    | 1:AA:641:U:H5'     | 2.08                     | 0.53              |
| 1:AA:672:U:H2'    | 1:AA:673:A:C8      | 2.43                     | 0.53              |
| 1:AA:711:G:O2'    | 1:AA:712:A:H5'     | 2.09                     | 0.53              |
| 7:AH:63:LYS:HG2   | 7:AH:70:VAL:HG21   | 1.90                     | 0.53              |
| 23:BB:136:G:H2'   | 23:BB:137:U:C5     | 2.43                     | 0.53              |
| 23:BB:197:A:N6    | 23:BB:2430:A:H2'   | 2.24                     | 0.53              |
| 23:BB:340:A:O2'   | 23:BB:341:C:H5'    | 2.08                     | 0.53              |
| 23:BB:633:A:O5'   | 23:BB:633:A:C8     | 2.57                     | 0.53              |
| 23:BB:737:C:O2'   | 23:BB:738:G:H5'    | 2.09                     | 0.53              |
| 23:BB:1745:A:O2'  | 23:BB:1746:A:H5'   | 2.09                     | 0.53              |
| 23:BB:1796:U:H2'  | 23:BB:1797:G:H8    | 1.73                     | 0.53              |
| 23:BB:2229:U:H2'  | 23:BB:2230:G:H8    | 1.74                     | 0.53              |
| 23:BB:2628:C:O2'  | 23:BB:2781:A:H2'   | 2.09                     | 0.53              |
| 24:BV:30:ILE:HD11 | 24:BV:63:ILE:HD12  | 1.90                     | 0.53              |
| 25:BC:16:VAL:O    | 25:BC:16:VAL:HG12  | 2.08                     | 0.53              |
| 27:BE:108:ILE:H   | 27:BE:108:ILE:HD12 | 1.73                     | 0.53              |
| 29:BG:29:ASN:N    | 29:BG:29:ASN:HD22  | 2.05                     | 0.53              |
| 29:BG:100:ASN:O   | 29:BG:115:GLN:HA   | 2.09                     | 0.53              |
| 37:BP:70:GLU:O    | 37:BP:71:ARG:HB2   | 2.08                     | 0.53              |
| 39:BR:39:LEU:HD12 | 39:BR:60:LYS:HB2   | 1.90                     | 0.53              |
| 42:BU:39:ASN:HD21 | 42:BU:42:LYS:HE2   | 1.71                     | 0.53              |
| 42:BU:59:GLU:O    | 42:BU:60:LYS:HB2   | 2.08                     | 0.53              |
| 42:BU:60:LYS:CG   | 42:BU:61:GLU:H     | 2.22                     | 0.53              |
| 43:BW:39:GLN:C    | 43:BW:40:ARG:HG3   | 2.33                     | 0.53              |
| 49:B2:25:LYS:H    | 49:B2:25:LYS:CE    | 2.21                     | 0.53              |
| 1:CA:764:C:C2'    | 1:CA:765:G:H5'     | 2.39                     | 0.53              |
| 1:CA:1158:C:O3'   | 20:CB:131:LYS:HD3  | 2.08                     | 0.53              |
| 1:CA:1277:C:H1'   | 1:CA:1282:C:O2     | 2.09                     | 0.53              |
| 1:CA:1311:A:N6    | 18:CS:1:PRO:HD3    | 2.21                     | 0.53              |
| 1:CA:1313:U:OP2   | 18:CS:5:LYS:HA     | 2.09                     | 0.53              |
| 2:CC:122:GLN:HB3  | 2:CC:127:VAL:HG11  | 1.89                     | 0.53              |
| 2:CC:166:TRP:HE1  | 2:CC:168:ARG:HB2   | 1.73                     | 0.53              |
| 4:CE:33:THR:HB    | 4:CE:49:TYR:CE1    | 2.43                     | 0.53              |
| 5:CF:9:MET:HB2    | 5:CF:57:ALA:HB1    | 1.90                     | 0.53              |
| 6:CG:59:GLU:HA    | 6:CG:62:GLU:CD     | 2.34                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:CH:71:VAL:O      | 7:CH:71:VAL:HG23  | 2.09                     | 0.53              |
| 16:CQ:16:MET:HB2   | 16:CQ:19:SER:HB2  | 1.91                     | 0.53              |
| 22:DA:10:G:H2'     | 22:DA:11:C:O4'    | 2.09                     | 0.53              |
| 23:DB:521:U:H2'    | 23:DB:522:A:C8    | 2.43                     | 0.53              |
| 23:DB:1138:G:H2'   | 23:DB:1139:G:O4'  | 2.09                     | 0.53              |
| 23:DB:1571:A:H2'   | 23:DB:1572:A:H8   | 1.73                     | 0.53              |
| 23:DB:1684:G:H2'   | 23:DB:1685:C:C6   | 2.44                     | 0.53              |
| 23:DB:2241:A:H2'   | 23:DB:2242:G:H8   | 1.72                     | 0.53              |
| 23:DB:2467:C:OP2   | 51:D4:7:VAL:HG12  | 2.09                     | 0.53              |
| 23:DB:2529:G:H5'   | 29:DG:175:LYS:HB3 | 1.89                     | 0.53              |
| 23:DB:2628:C:O2'   | 23:DB:2781:A:H2'  | 2.09                     | 0.53              |
| 24:DV:63:ILE:N     | 24:DV:63:ILE:HD12 | 2.24                     | 0.53              |
| 25:DC:53:ILE:CD1   | 25:DC:218:THR:HA  | 2.39                     | 0.53              |
| 25:DC:268:ARG:O    | 25:DC:269:ARG:HB2 | 2.09                     | 0.53              |
| 26:DD:46:ARG:HH21  | 26:DD:80:TRP:CD1  | 2.26                     | 0.53              |
| 27:DE:14:VAL:HG11  | 27:DE:16:GLU:CD   | 2.34                     | 0.53              |
| 27:DE:189:THR:HG23 | 27:DE:194:LYS:HB2 | 1.89                     | 0.53              |
| 29:DG:3:VAL:O      | 29:DG:4:ALA:HB2   | 2.08                     | 0.53              |
| 30:DH:94:ILE:HG23  | 30:DH:98:ASP:HB2  | 1.90                     | 0.53              |
| 32:DK:41:ILE:HG13  | 32:DK:42:THR:H    | 1.74                     | 0.53              |
| 33:DL:50:PHE:O     | 33:DL:51:GLU:C    | 2.51                     | 0.53              |
| 33:DL:109:LYS:HG2  | 33:DL:126:ARG:CD  | 2.38                     | 0.53              |
| 34:DM:33:LEU:HG    | 34:DM:113:ALA:HB1 | 1.91                     | 0.53              |
| 35:DN:29:VAL:HG21  | 35:DN:75:ILE:HB   | 1.90                     | 0.53              |
| 35:DN:107:ASN:ND2  | 40:DS:40:ASN:HB3  | 2.23                     | 0.53              |
| 43:DW:73:PRO:C     | 43:DW:74:LYS:HD2  | 2.34                     | 0.53              |
| 44:DX:7:ARG:HB3    | 44:DX:7:ARG:NH1   | 2.24                     | 0.53              |
| 44:DX:55:THR:C     | 44:DX:57:LEU:H    | 2.15                     | 0.53              |
| 1:AA:44:A:O2'      | 1:AA:45:G:H5'     | 2.09                     | 0.53              |
| 1:AA:476:U:H2'     | 1:AA:477:C:H6     | 1.73                     | 0.53              |
| 1:AA:963:G:H21     | 9:AJ:56:HIS:HE1   | 1.55                     | 0.53              |
| 10:AK:105:ARG:NH2  | 21:AU:10:PRO:HG3  | 2.24                     | 0.53              |
| 11:AL:28:GLN:HG3   | 11:AL:80:LEU:HD21 | 1.90                     | 0.53              |
| 13:AN:51:PRO:HB2   | 13:AN:54:SER:HB3  | 1.91                     | 0.53              |
| 23:BB:184:C:H2'    | 23:BB:185:G:H8    | 1.72                     | 0.53              |
| 23:BB:337:C:H2'    | 23:BB:338:G:O4'   | 2.09                     | 0.53              |
| 23:BB:1549:A:H2'   | 23:BB:1550:C:C6   | 2.44                     | 0.53              |
| 23:BB:1826:G:H2'   | 23:BB:1827:U:C6   | 2.44                     | 0.53              |
| 23:BB:1846:G:H2'   | 23:BB:1847:A:O4'  | 2.09                     | 0.53              |
| 23:BB:2213:U:O2    | 23:BB:2213:U:H2'  | 2.07                     | 0.53              |
| 23:BB:2263:C:H2'   | 23:BB:2264:C:H6   | 1.74                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:2308:G:N3    | 23:BB:2308:G:H5''  | 2.24                     | 0.53              |
| 23:BB:2820:A:O5'   | 35:BN:4:ARG:HA     | 2.08                     | 0.53              |
| 26:BD:109:VAL:HG11 | 26:BD:193:VAL:HG23 | 1.90                     | 0.53              |
| 29:BG:163:TYR:HB2  | 29:BG:166:GLU:HB2  | 1.90                     | 0.53              |
| 31:BJ:101:ILE:HG23 | 31:BJ:102:GLU:OE1  | 2.08                     | 0.53              |
| 34:BM:114:ARG:HA   | 34:BM:117:PHE:HB3  | 1.91                     | 0.53              |
| 35:BN:57:THR:HG23  | 35:BN:58:ASP:H     | 1.74                     | 0.53              |
| 38:BQ:92:LYS:HE3   | 38:BQ:93:ILE:HB    | 1.91                     | 0.53              |
| 44:BX:14:LEU:O     | 44:BX:17:GLU:HB2   | 2.09                     | 0.53              |
| 47:B0:11:LYS:C     | 47:B0:13:GLY:H     | 2.15                     | 0.53              |
| 51:B4:14:CYS:SG    | 51:B4:27:CYS:HB3   | 2.48                     | 0.53              |
| 1:CA:462:G:H2'     | 1:CA:463:U:C6      | 2.44                     | 0.53              |
| 1:CA:975:A:C2'     | 1:CA:976:G:OP2     | 2.57                     | 0.53              |
| 2:CC:63:ILE:HG12   | 2:CC:65:VAL:HG23   | 1.91                     | 0.53              |
| 3:CD:27:ILE:C      | 3:CD:29:THR:H      | 2.16                     | 0.53              |
| 3:CD:170:LEU:HA    | 3:CD:182:LYS:HG3   | 1.91                     | 0.53              |
| 18:CS:28:LYS:HB3   | 18:CS:28:LYS:NZ    | 2.23                     | 0.53              |
| 23:DB:18:U:H2'     | 23:DB:19:A:H8      | 1.74                     | 0.53              |
| 23:DB:443:A:H5''   | 23:DB:444:C:OP1    | 2.09                     | 0.53              |
| 23:DB:544:C:H2'    | 23:DB:545:U:N3     | 2.24                     | 0.53              |
| 23:DB:632:A:O3'    | 33:DL:69:ARG:HD3   | 2.09                     | 0.53              |
| 23:DB:766:U:H2'    | 23:DB:767:U:C6     | 2.44                     | 0.53              |
| 23:DB:934:U:H2'    | 23:DB:935:C:C6     | 2.44                     | 0.53              |
| 23:DB:1105:U:H2'   | 23:DB:1106:G:C8    | 2.41                     | 0.53              |
| 23:DB:1430:G:H2'   | 23:DB:1431:A:H8    | 1.74                     | 0.53              |
| 23:DB:2028:U:H2'   | 23:DB:2029:G:C8    | 2.44                     | 0.53              |
| 23:DB:2886:A:C5    | 47:D0:27:LEU:HG    | 2.43                     | 0.53              |
| 24:DV:1:MET:SD     | 24:DV:62:THR:HG23  | 2.49                     | 0.53              |
| 25:DC:32:LEU:HD23  | 25:DC:32:LEU:N     | 2.23                     | 0.53              |
| 25:DC:124:LYS:HB2  | 25:DC:125:PRO:CD   | 2.39                     | 0.53              |
| 25:DC:231:HIS:HD1  | 25:DC:242:HIS:HA   | 1.74                     | 0.53              |
| 28:DF:39:VAL:HG13  | 28:DF:84:ILE:CG1   | 2.39                     | 0.53              |
| 28:DF:177:ARG:CZ   | 28:DF:178:LYS:HA   | 2.39                     | 0.53              |
| 43:DW:42:THR:N     | 43:DW:65:LYS:HG2   | 2.23                     | 0.53              |
| 45:DY:50:VAL:CG1   | 45:DY:53:MET:HG2   | 2.39                     | 0.53              |
| 46:DZ:41:HIS:O     | 46:DZ:43:PHE:HD1   | 1.92                     | 0.53              |
| 52:DI:90:GLY:C     | 52:DI:92:PRO:HD3   | 2.34                     | 0.53              |
| 1:AA:588:G:H5'     | 7:AH:2:MET:O       | 2.09                     | 0.53              |
| 1:AA:777:A:H2'     | 1:AA:778:G:C8      | 2.43                     | 0.53              |
| 1:AA:1033:G:H3'    | 1:AA:1034:G:H5''   | 1.91                     | 0.53              |
| 1:AA:1392:G:H2'    | 1:AA:1393:U:C6     | 2.44                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:AC:90:VAL:HG23   | 2:AC:98:ALA:HB3    | 1.90                     | 0.53              |
| 2:AC:119:ILE:O     | 2:AC:123:LEU:HG    | 2.09                     | 0.53              |
| 5:AF:3:HIS:HB2     | 5:AF:92:THR:OG1    | 2.09                     | 0.53              |
| 6:AG:143:MET:O     | 6:AG:147:ASN:HB2   | 2.09                     | 0.53              |
| 16:AQ:17:GLU:C     | 16:AQ:19:SER:H     | 2.17                     | 0.53              |
| 16:AQ:45:VAL:HG11  | 16:AQ:74:LEU:HB2   | 1.90                     | 0.53              |
| 16:AQ:57:VAL:HB    | 16:AQ:79:GLU:H     | 1.74                     | 0.53              |
| 16:AQ:68:LYS:O     | 16:AQ:69:THR:HB    | 2.09                     | 0.53              |
| 22:BA:78:A:H2'     | 22:BA:79:G:O4'     | 2.09                     | 0.53              |
| 23:BB:503:A:C3'    | 23:BB:504:A:H5'    | 2.39                     | 0.53              |
| 23:BB:2484:G:O2'   | 34:BM:45:GLN:NE2   | 2.41                     | 0.53              |
| 23:BB:2688:G:H1'   | 23:BB:2721:A:H61   | 1.74                     | 0.53              |
| 23:BB:2898:U:H2'   | 23:BB:2899:A:C8    | 2.44                     | 0.53              |
| 25:BC:19:VAL:HG12  | 25:BC:20:ASN:N     | 2.15                     | 0.53              |
| 28:BF:4:HIS:O      | 28:BF:7:TYR:HB3    | 2.09                     | 0.53              |
| 28:BF:55:ASP:CG    | 28:BF:148:VAL:HG11 | 2.34                     | 0.53              |
| 29:BG:25:ILE:O     | 29:BG:31:GLU:HA    | 2.09                     | 0.53              |
| 29:BG:102:ILE:O    | 29:BG:113:ASP:HA   | 2.08                     | 0.53              |
| 34:BM:65:ILE:HA    | 34:BM:101:VAL:HA   | 1.90                     | 0.53              |
| 35:BN:118:ARG:O    | 35:BN:118:ARG:HG3  | 2.09                     | 0.53              |
| 36:BO:46:GLU:C     | 36:BO:48:LEU:H     | 2.17                     | 0.53              |
| 36:BO:62:LEU:HD12  | 36:BO:64:TYR:HB2   | 1.90                     | 0.53              |
| 40:BS:20:VAL:O     | 40:BS:23:LEU:HB2   | 2.09                     | 0.53              |
| 40:BS:86:MET:SD    | 40:BS:96:ILE:HD11  | 2.49                     | 0.53              |
| 43:BW:16:GLU:O     | 43:BW:18:LYS:HD2   | 2.09                     | 0.53              |
| 1:CA:203:G:N2      | 1:CA:205:A:N6      | 2.56                     | 0.53              |
| 1:CA:556:C:O2'     | 1:CA:557:G:H5'     | 2.08                     | 0.53              |
| 1:CA:640:A:O2'     | 1:CA:641:U:H5'     | 2.08                     | 0.53              |
| 1:CA:858:G:O6      | 1:CA:869:G:H3'     | 2.09                     | 0.53              |
| 1:CA:883:C:O2'     | 1:CA:884:U:H5'     | 2.09                     | 0.53              |
| 1:CA:1478:U:H2'    | 1:CA:1479:C:C6     | 2.43                     | 0.53              |
| 2:CC:23:ALA:HB1    | 2:CC:27:GLU:HB2    | 1.91                     | 0.53              |
| 2:CC:53:ARG:HA     | 2:CC:113:LYS:NZ    | 2.23                     | 0.53              |
| 2:CC:91:ALA:HB2    | 2:CC:98:ALA:HB3    | 1.90                     | 0.53              |
| 15:CP:44:SER:CB    | 15:CP:46:LYS:HG2   | 2.35                     | 0.53              |
| 20:CB:16:GLY:CA    | 20:CB:40:ILE:H     | 2.21                     | 0.53              |
| 20:CB:53:LEU:HD13  | 20:CB:212:TYR:OH   | 2.09                     | 0.53              |
| 20:CB:150:ILE:HG12 | 20:CB:150:ILE:O    | 2.09                     | 0.53              |
| 20:CB:153:MET:C    | 20:CB:155:GLY:H    | 2.17                     | 0.53              |
| 23:DB:228:C:H4'    | 23:DB:229:C:H5''   | 1.90                     | 0.53              |
| 23:DB:250:G:C5'    | 50:D3:7:ARG:HG2    | 2.35                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:1368:G:OP1   | 49:D2:25:LYS:HG3   | 2.09                     | 0.53              |
| 23:DB:1594:U:H2'   | 23:DB:1595:C:H6    | 1.74                     | 0.53              |
| 23:DB:1846:G:H2'   | 23:DB:1847:A:O4'   | 2.09                     | 0.53              |
| 23:DB:2313:C:H5'   | 28:DF:36:ASN:ND2   | 2.23                     | 0.53              |
| 23:DB:2489:U:O2'   | 23:DB:2490:G:H5'   | 2.08                     | 0.53              |
| 23:DB:2512:C:H2'   | 23:DB:2513:A:O4'   | 2.08                     | 0.53              |
| 23:DB:2634:A:H2'   | 23:DB:2635:A:C8    | 2.44                     | 0.53              |
| 24:DV:53:LYS:NZ    | 24:DV:55:GLU:HG2   | 2.23                     | 0.53              |
| 26:DD:149:ASN:H    | 26:DD:151:THR:HG23 | 1.73                     | 0.53              |
| 26:DD:153:GLY:C    | 26:DD:155:VAL:N    | 2.65                     | 0.53              |
| 27:DE:1:MET:HE2    | 27:DE:1:MET:N      | 2.24                     | 0.53              |
| 31:DJ:109:LEU:HD22 | 31:DJ:115:GLY:O    | 2.09                     | 0.53              |
| 37:DP:89:GLY:HA2   | 37:DP:112:ARG:NH2  | 2.23                     | 0.53              |
| 39:DR:32:THR:HB    | 39:DR:65:ALA:C     | 2.34                     | 0.53              |
| 47:D0:51:ARG:O     | 47:D0:51:ARG:HD3   | 2.08                     | 0.53              |
| 1:AA:537:G:H2'     | 1:AA:538:G:H8      | 1.74                     | 0.52              |
| 4:AE:156:ARG:HB2   | 7:AH:43:GLY:HA3    | 1.91                     | 0.52              |
| 6:AG:130:LYS:N     | 6:AG:134:VAL:HG11  | 2.23                     | 0.52              |
| 8:AI:115:VAL:HG21  | 9:AJ:62:ARG:HB2    | 1.90                     | 0.52              |
| 12:AM:27:THR:O     | 12:AM:30:LYS:HB3   | 2.09                     | 0.52              |
| 18:AS:66:VAL:C     | 18:AS:68:HIS:H     | 2.17                     | 0.52              |
| 19:AT:28:ARG:HA    | 19:AT:31:ILE:HD12  | 1.91                     | 0.52              |
| 20:AB:30:ILE:HG22  | 20:AB:32:GLY:H     | 1.74                     | 0.52              |
| 23:BB:877:A:N1     | 23:BB:900:A:N7     | 2.57                     | 0.52              |
| 23:BB:1050:A:H2'   | 23:BB:1051:G:O4'   | 2.10                     | 0.52              |
| 23:BB:1183:U:H2'   | 23:BB:1184:U:C6    | 2.43                     | 0.52              |
| 23:BB:1844:C:OP1   | 25:BC:252:LYS:HA   | 2.09                     | 0.52              |
| 23:BB:2144:G:N2    | 23:BB:2148:G:N3    | 2.57                     | 0.52              |
| 23:BB:2218:G:H2'   | 23:BB:2219:U:H6    | 1.73                     | 0.52              |
| 23:BB:2305:U:H2'   | 23:BB:2306:C:C6    | 2.43                     | 0.52              |
| 23:BB:2675:A:N1    | 23:BB:2732:G:O6    | 2.42                     | 0.52              |
| 27:BE:144:GLU:HG3  | 27:BE:145:ASP:H    | 1.73                     | 0.52              |
| 28:BF:106:ALA:HB1  | 28:BF:136:ILE:HG23 | 1.90                     | 0.52              |
| 33:BL:56:PRO:O     | 33:BL:59:ARG:HB2   | 2.08                     | 0.52              |
| 33:BL:106:GLU:HG2  | 33:BL:107:PHE:H    | 1.74                     | 0.52              |
| 33:BL:126:ARG:HH21 | 33:BL:131:ALA:HB2  | 1.73                     | 0.52              |
| 34:BM:7:THR:O      | 34:BM:8:LYS:HD3    | 2.09                     | 0.52              |
| 34:BM:15:GLY:O     | 34:BM:16:ARG:HB3   | 2.09                     | 0.52              |
| 37:BP:29:VAL:C     | 37:BP:44:GLY:HA3   | 2.34                     | 0.52              |
| 38:BQ:84:LYS:HE3   | 38:BQ:84:LYS:N     | 2.24                     | 0.52              |
| 38:BQ:88:GLU:HG2   | 39:BR:53:PHE:CD2   | 2.45                     | 0.52              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:BR:63:VAL:HB    | 39:BR:101:ILE:HG12 | 1.91                     | 0.52              |
| 40:BS:11:ARG:O     | 40:BS:11:ARG:HD3   | 2.08                     | 0.52              |
| 41:BT:20:ALA:C     | 41:BT:22:THR:H     | 2.17                     | 0.52              |
| 42:BU:35:VAL:C     | 42:BU:36:GLU:HG2   | 2.34                     | 0.52              |
| 44:BX:29:ARG:CA    | 44:BX:34:SER:HB2   | 2.39                     | 0.52              |
| 48:B1:42:VAL:O     | 48:B1:43:ARG:HB2   | 2.09                     | 0.52              |
| 1:CA:113:G:H2'     | 1:CA:114:U:C6      | 2.44                     | 0.52              |
| 1:CA:1142:G:H2'    | 1:CA:1143:G:C8     | 2.44                     | 0.52              |
| 1:CA:1171:A:H2'    | 1:CA:1172:C:C6     | 2.44                     | 0.52              |
| 1:CA:1244:G:H2'    | 1:CA:1245:C:H6     | 1.71                     | 0.52              |
| 2:CC:151:GLU:HA    | 2:CC:166:TRP:HA    | 1.90                     | 0.52              |
| 4:CE:156:ARG:HD2   | 7:CH:42:GLU:O      | 2.09                     | 0.52              |
| 5:CF:25:TYR:O      | 5:CF:29:ILE:HG13   | 2.09                     | 0.52              |
| 8:CI:56:MET:C      | 8:CI:58:GLU:H      | 2.17                     | 0.52              |
| 10:CK:48:GLY:C     | 10:CK:50:GLY:H     | 2.17                     | 0.52              |
| 13:CN:43:ALA:O     | 13:CN:47:LEU:HB2   | 2.09                     | 0.52              |
| 16:CQ:60:ILE:HD13  | 16:CQ:60:ILE:H     | 1.74                     | 0.52              |
| 19:CT:2:ASN:O      | 19:CT:3:ILE:C      | 2.52                     | 0.52              |
| 21:CU:6:ARG:C      | 21:CU:7:GLU:HG2    | 2.34                     | 0.52              |
| 23:DB:204:A:H4'    | 23:DB:205:G:OP1    | 2.09                     | 0.52              |
| 23:DB:929:U:H1'    | 45:DY:24:LEU:O     | 2.09                     | 0.52              |
| 23:DB:1042:G:H2'   | 23:DB:1043:C:C6    | 2.45                     | 0.52              |
| 23:DB:1060:U:O2    | 23:DB:1088:A:C8    | 2.63                     | 0.52              |
| 23:DB:1186:G:H2'   | 23:DB:1187:G:O4'   | 2.09                     | 0.52              |
| 23:DB:1864:U:O2'   | 23:DB:1865:U:H5'   | 2.08                     | 0.52              |
| 23:DB:2047:C:H2'   | 23:DB:2048:G:H8    | 1.74                     | 0.52              |
| 25:DC:37:SER:H     | 25:DC:62:ARG:CB    | 2.21                     | 0.52              |
| 25:DC:181:ARG:O    | 25:DC:181:ARG:HG3  | 2.09                     | 0.52              |
| 27:DE:120:VAL:HG12 | 27:DE:121:VAL:N    | 2.18                     | 0.52              |
| 28:DF:39:VAL:HG13  | 28:DF:84:ILE:HB    | 1.91                     | 0.52              |
| 33:DL:69:ARG:HG3   | 33:DL:71:ALA:O     | 2.09                     | 0.52              |
| 33:DL:90:VAL:CG1   | 33:DL:122:VAL:HG22 | 2.39                     | 0.52              |
| 33:DL:92:LEU:HA    | 33:DL:96:LYS:HG2   | 1.91                     | 0.52              |
| 48:D1:42:VAL:O     | 48:D1:43:ARG:HB2   | 2.06                     | 0.52              |
| 51:D4:19:ARG:HH11  | 51:D4:19:ARG:HB3   | 1.73                     | 0.52              |
| 1:AA:1115:U:H2'    | 1:AA:1116:U:C6     | 2.45                     | 0.52              |
| 1:AA:1438:G:O2'    | 1:AA:1439:G:H5'    | 2.08                     | 0.52              |
| 6:AG:16:LYS:HG3    | 6:AG:43:TYR:OH     | 2.08                     | 0.52              |
| 6:AG:85:GLN:O      | 6:AG:86:VAL:C      | 2.52                     | 0.52              |
| 9:AJ:5:ARG:HD3     | 9:AJ:5:ARG:N       | 2.24                     | 0.52              |
| 13:AN:81:ILE:O     | 13:AN:84:ARG:HB3   | 2.09                     | 0.52              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:AQ:45:VAL:HG12 | 16:AQ:46:HIS:N    | 2.21                     | 0.52              |
| 20:AB:160:LEU:O   | 20:AB:182:VAL:HA  | 2.09                     | 0.52              |
| 23:BB:49:A:OP1    | 23:BB:49:A:H4'    | 2.09                     | 0.52              |
| 23:BB:154:U:H2'   | 23:BB:155:A:H8    | 1.74                     | 0.52              |
| 23:BB:279:A:N1    | 23:BB:362:A:H5'   | 2.24                     | 0.52              |
| 23:BB:328:U:H4'   | 42:BU:65:GLN:HE21 | 1.74                     | 0.52              |
| 23:BB:1151:A:H2'  | 23:BB:1152:C:H6   | 1.74                     | 0.52              |
| 23:BB:1664:A:H1'  | 23:BB:2726:A:N1   | 2.23                     | 0.52              |
| 23:BB:2213:U:H2'  | 23:BB:2214:C:H5'  | 1.92                     | 0.52              |
| 23:BB:2348:U:O2'  | 23:BB:2349:G:H5'  | 2.09                     | 0.52              |
| 23:BB:2649:C:H2'  | 23:BB:2650:U:H6   | 1.73                     | 0.52              |
| 23:BB:2750:A:H3'  | 29:BG:3:VAL:HG13  | 1.90                     | 0.52              |
| 23:BB:2849:U:O4   | 37:BP:96:LEU:HD21 | 2.09                     | 0.52              |
| 25:BC:81:GLU:HB3  | 25:BC:90:ILE:CG2  | 2.40                     | 0.52              |
| 26:BD:15:PHE:HB3  | 26:BD:18:ASP:HB3  | 1.90                     | 0.52              |
| 30:BH:41:LYS:HD2  | 30:BH:41:LYS:H    | 1.74                     | 0.52              |
| 31:BJ:114:LEU:O   | 31:BJ:117:ALA:HB3 | 2.10                     | 0.52              |
| 34:BM:32:GLY:HA2  | 34:BM:101:VAL:O   | 2.09                     | 0.52              |
| 35:BN:12:ARG:HD3  | 35:BN:20:MET:HE3  | 1.90                     | 0.52              |
| 37:BP:47:ILE:HG23 | 37:BP:63:ILE:HG23 | 1.91                     | 0.52              |
| 38:BQ:50:ARG:HA   | 38:BQ:53:LYS:CE   | 2.39                     | 0.52              |
| 40:BS:29:VAL:C    | 40:BS:31:GLN:H    | 2.16                     | 0.52              |
| 41:BT:3:ARG:HG2   | 41:BT:7:LEU:HB3   | 1.92                     | 0.52              |
| 52:BI:81:LYS:HG3  | 52:BI:82:ALA:N    | 2.24                     | 0.52              |
| 1:CA:685:G:O2'    | 1:CA:686:U:H5'    | 2.09                     | 0.52              |
| 1:CA:1337:G:H5''  | 1:CA:1338:G:OP1   | 2.09                     | 0.52              |
| 1:CA:1480:A:H2'   | 1:CA:1481:U:C6    | 2.43                     | 0.52              |
| 5:CF:38:ARG:NH1   | 5:CF:98:GLU:H     | 1.98                     | 0.52              |
| 5:CF:85:ILE:HG22  | 5:CF:86:ARG:H     | 1.73                     | 0.52              |
| 9:CJ:41:PRO:HA    | 9:CJ:72:ARG:CD    | 2.38                     | 0.52              |
| 13:CN:5:MET:HA    | 13:CN:8:ARG:HG3   | 1.92                     | 0.52              |
| 16:CQ:10:ARG:CZ   | 16:CQ:11:VAL:H    | 2.22                     | 0.52              |
| 18:CS:43:MET:HB3  | 18:CS:61:VAL:HG11 | 1.91                     | 0.52              |
| 20:CB:23:ASN:HD22 | 20:CB:24:PRO:CD   | 2.22                     | 0.52              |
| 22:DA:87:U:O2'    | 22:DA:88:C:H2'    | 2.08                     | 0.52              |
| 23:DB:178:G:O2'   | 23:DB:179:C:H5'   | 2.09                     | 0.52              |
| 23:DB:323:C:H5    | 27:DE:165:HIS:HB2 | 1.74                     | 0.52              |
| 23:DB:997:G:OP1   | 38:DQ:92:LYS:HB3  | 2.09                     | 0.52              |
| 23:DB:1754:A:OP1  | 37:DP:95:LYS:HB2  | 2.10                     | 0.52              |
| 23:DB:1911:U:H2'  | 23:DB:1918:A:N1   | 2.22                     | 0.52              |
| 23:DB:2359:C:H4'  | 50:D3:51:LYS:HD2  | 1.91                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:DC:136:VAL:C   | 25:DC:165:ALA:HA   | 2.34                     | 0.52              |
| 30:DH:26:ALA:C    | 30:DH:28:ASN:H     | 2.16                     | 0.52              |
| 30:DH:135:HIS:CD2 | 30:DH:137:GLU:H    | 2.26                     | 0.52              |
| 31:DJ:67:ASN:C    | 31:DJ:69:ARG:H     | 2.16                     | 0.52              |
| 37:DP:7:LEU:CD2   | 37:DP:11:GLN:HE21  | 2.22                     | 0.52              |
| 37:DP:77:SER:HB2  | 37:DP:78:PRO:HD3   | 1.90                     | 0.52              |
| 37:DP:91:VAL:HG23 | 37:DP:113:LEU:HB3  | 1.92                     | 0.52              |
| 38:DQ:26:ALA:CA   | 38:DQ:30:VAL:HG23  | 2.39                     | 0.52              |
| 48:D1:10:LEU:HD13 | 48:D1:50:GLU:OE1   | 2.10                     | 0.52              |
| 50:D3:33:THR:CG2  | 50:D3:40:LYS:HD2   | 2.38                     | 0.52              |
| 1:AA:214:C:H2'    | 1:AA:215:C:H6      | 1.72                     | 0.52              |
| 1:AA:333:U:H2'    | 1:AA:334:C:H6      | 1.74                     | 0.52              |
| 1:AA:392:C:H2'    | 1:AA:393:A:H8      | 1.75                     | 0.52              |
| 1:AA:552:U:H4'    | 11:AL:82:ARG:HG2   | 1.92                     | 0.52              |
| 1:AA:556:C:O2'    | 1:AA:557:G:H5'     | 2.08                     | 0.52              |
| 1:AA:858:G:O6     | 1:AA:869:G:H3'     | 2.09                     | 0.52              |
| 2:AC:71:ARG:HB3   | 2:AC:74:ILE:HG22   | 1.92                     | 0.52              |
| 2:AC:78:LYS:O     | 2:AC:78:LYS:HG3    | 2.10                     | 0.52              |
| 5:AF:88:MET:HE2   | 5:AF:89:VAL:N      | 2.25                     | 0.52              |
| 8:AI:47:VAL:HG12  | 8:AI:78:ILE:HB     | 1.91                     | 0.52              |
| 8:AI:48:ARG:HA    | 8:AI:51:LEU:HD13   | 1.92                     | 0.52              |
| 9:AJ:56:HIS:N     | 13:AN:80:ARG:HH22  | 2.07                     | 0.52              |
| 23:BB:522:A:H2'   | 23:BB:523:C:C6     | 2.45                     | 0.52              |
| 23:BB:600:G:H2'   | 23:BB:601:C:C6     | 2.45                     | 0.52              |
| 23:BB:995:C:N4    | 31:BJ:2:LYS:HB3    | 2.25                     | 0.52              |
| 23:BB:1010:A:H5'  | 38:BQ:61:ILE:HD12  | 1.91                     | 0.52              |
| 23:BB:2028:U:H2'  | 23:BB:2029:G:C8    | 2.44                     | 0.52              |
| 23:BB:2579:C:O2'  | 26:BD:138:LEU:HD13 | 2.10                     | 0.52              |
| 23:BB:2618:G:O2'  | 26:BD:154:LYS:O    | 2.26                     | 0.52              |
| 23:BB:2719:G:H4'  | 23:BB:2846:G:O3'   | 2.09                     | 0.52              |
| 24:BV:14:LYS:HZ2  | 24:BV:18:ARG:HD2   | 1.72                     | 0.52              |
| 25:BC:46:GLY:O    | 25:BC:47:ARG:CB    | 2.56                     | 0.52              |
| 25:BC:53:ILE:HD13 | 25:BC:218:THR:CG2  | 2.30                     | 0.52              |
| 25:BC:114:GLN:HB2 | 25:BC:124:LYS:NZ   | 2.24                     | 0.52              |
| 31:BJ:34:ARG:HB3  | 31:BJ:39:LYS:HD2   | 1.91                     | 0.52              |
| 32:BK:41:ILE:HG23 | 32:BK:42:THR:N     | 2.24                     | 0.52              |
| 39:BR:90:ARG:NH1  | 39:BR:91:GLN:H     | 2.08                     | 0.52              |
| 1:CA:394:G:H2'    | 1:CA:395:C:H6      | 1.75                     | 0.52              |
| 1:CA:537:G:H2'    | 1:CA:538:G:H8      | 1.75                     | 0.52              |
| 1:CA:625:U:H4'    | 15:CP:16:PHE:CE2   | 2.44                     | 0.52              |
| 1:CA:663:A:O2'    | 1:CA:664:G:H5'     | 2.10                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1000:A:H2'   | 1:CA:1001:C:H6     | 1.71                     | 0.52              |
| 1:CA:1049:U:O2'   | 1:CA:1050:G:OP2    | 2.26                     | 0.52              |
| 1:CA:1057:G:H5''  | 2:CC:153:SER:HB2   | 1.91                     | 0.52              |
| 1:CA:1060:U:C4'   | 9:CJ:54:SER:HB2    | 2.39                     | 0.52              |
| 1:CA:1330:U:OP1   | 12:CM:22:TYR:O     | 2.27                     | 0.52              |
| 3:CD:118:SER:C    | 3:CD:120:LYS:H     | 2.18                     | 0.52              |
| 3:CD:171:GLU:HG3  | 3:CD:182:LYS:CD    | 2.39                     | 0.52              |
| 4:CE:35:LEU:CD1   | 4:CE:133:ILE:HA    | 2.40                     | 0.52              |
| 5:CF:3:HIS:NE2    | 5:CF:95:ALA:HB2    | 2.24                     | 0.52              |
| 5:CF:38:ARG:NH2   | 5:CF:63:ASN:HD21   | 2.07                     | 0.52              |
| 6:CG:77:ARG:HD3   | 6:CG:79:VAL:HG23   | 1.92                     | 0.52              |
| 6:CG:145:GLU:H    | 6:CG:148:LYS:HB2   | 1.75                     | 0.52              |
| 10:CK:109:ILE:H   | 10:CK:109:ILE:HD12 | 1.74                     | 0.52              |
| 13:CN:31:SER:O    | 13:CN:40:ARG:HD3   | 2.09                     | 0.52              |
| 18:CS:62:THR:HG22 | 18:CS:65:MET:HE3   | 1.91                     | 0.52              |
| 23:DB:18:U:H2'    | 23:DB:19:A:C8      | 2.44                     | 0.52              |
| 23:DB:19:A:H2'    | 23:DB:20:C:C6      | 2.44                     | 0.52              |
| 23:DB:19:A:H2'    | 23:DB:20:C:H6      | 1.75                     | 0.52              |
| 23:DB:20:C:O2'    | 23:DB:21:A:H5'     | 2.09                     | 0.52              |
| 23:DB:136:G:C2    | 41:DT:3:ARG:NH2    | 2.77                     | 0.52              |
| 23:DB:324:A:N6    | 23:DB:339:U:H5'    | 2.24                     | 0.52              |
| 23:DB:599:A:N3    | 27:DE:100:MET:HE1  | 2.24                     | 0.52              |
| 23:DB:664:G:H2'   | 23:DB:665:U:C6     | 2.43                     | 0.52              |
| 23:DB:721:A:H2'   | 23:DB:722:A:H8     | 1.74                     | 0.52              |
| 23:DB:1034:G:H2'  | 23:DB:1035:U:C6    | 2.43                     | 0.52              |
| 23:DB:1374:G:H2'  | 23:DB:1375:U:C6    | 2.45                     | 0.52              |
| 23:DB:1733:G:H2'  | 23:DB:1734:G:C8    | 2.45                     | 0.52              |
| 23:DB:2675:A:N1   | 23:DB:2732:G:O6    | 2.42                     | 0.52              |
| 23:DB:2734:A:H2'  | 23:DB:2735:G:H5'   | 1.91                     | 0.52              |
| 32:DK:71:ARG:CB   | 32:DK:72:PRO:CD    | 2.87                     | 0.52              |
| 33:DL:108:ALA:O   | 33:DL:109:LYS:HB2  | 2.09                     | 0.52              |
| 37:DP:52:ARG:CB   | 37:DP:60:VAL:HG11  | 2.36                     | 0.52              |
| 39:DR:26:ASP:O    | 39:DR:27:ILE:HB    | 2.09                     | 0.52              |
| 42:DU:21:ARG:HG3  | 42:DU:21:ARG:NH1   | 2.23                     | 0.52              |
| 51:D4:7:VAL:O     | 51:D4:8:LYS:HB2    | 2.08                     | 0.52              |
| 1:AA:317:U:H2'    | 1:AA:318:G:H8      | 1.73                     | 0.52              |
| 1:AA:1225:A:H3'   | 1:AA:1226:C:H6     | 1.74                     | 0.52              |
| 1:AA:1390:U:H2'   | 1:AA:1391:U:C6     | 2.44                     | 0.52              |
| 5:AF:68:GLN:O     | 5:AF:71:ILE:HG13   | 2.09                     | 0.52              |
| 6:AG:13:PRO:HA    | 6:AG:23:ALA:HB2    | 1.90                     | 0.52              |
| 7:AH:64:TYR:CB    | 7:AH:69:ALA:HA     | 2.38                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:AI:61:ASP:O      | 8:AI:62:LEU:HD13   | 2.09                     | 0.52              |
| 17:AR:31:TYR:CD2   | 17:AR:54:LEU:HD21  | 2.45                     | 0.52              |
| 20:AB:163:ILE:HD11 | 20:AB:209:VAL:HG12 | 1.92                     | 0.52              |
| 22:BA:54:G:H2'     | 22:BA:55:U:C6      | 2.44                     | 0.52              |
| 23:BB:143:C:O2'    | 41:BT:5:GLU:HA     | 2.09                     | 0.52              |
| 23:BB:175:G:H2'    | 23:BB:176:A:C8     | 2.45                     | 0.52              |
| 23:BB:766:U:H2'    | 23:BB:767:U:C6     | 2.45                     | 0.52              |
| 23:BB:1242:U:H2'   | 23:BB:1243:C:C6    | 2.44                     | 0.52              |
| 23:BB:1739:A:H2'   | 23:BB:1740:G:O4'   | 2.10                     | 0.52              |
| 23:BB:2386:A:H4'   | 43:BW:38:ARG:HB2   | 1.91                     | 0.52              |
| 23:BB:2553:G:H2'   | 23:BB:2554:U:H4'   | 1.90                     | 0.52              |
| 23:BB:2734:A:H2'   | 23:BB:2735:G:H5'   | 1.91                     | 0.52              |
| 23:BB:2741:A:H2'   | 23:BB:2742:G:O4'   | 2.08                     | 0.52              |
| 25:BC:49:THR:O     | 25:BC:50:THR:HB    | 2.10                     | 0.52              |
| 32:BK:101:GLY:O    | 32:BK:119:ALA:HB1  | 2.08                     | 0.52              |
| 33:BL:30:THR:HA    | 33:BL:36:LYS:CE    | 2.37                     | 0.52              |
| 38:BQ:99:VAL:HG23  | 38:BQ:100:PHE:HD1  | 1.73                     | 0.52              |
| 42:BU:100:GLU:O    | 42:BU:102:ILE:HG13 | 2.10                     | 0.52              |
| 43:BW:36:ILE:HB    | 43:BW:68:PHE:CD2   | 2.41                     | 0.52              |
| 1:CA:1302:C:H5''   | 1:CA:1303:C:OP2    | 2.10                     | 0.52              |
| 4:CE:80:LEU:HD23   | 4:CE:122:VAL:HG11  | 1.91                     | 0.52              |
| 13:CN:60:ARG:O     | 13:CN:61:ASN:HB2   | 2.09                     | 0.52              |
| 14:CO:61:GLN:O     | 14:CO:65:LEU:HG    | 2.08                     | 0.52              |
| 18:CS:18:VAL:C     | 18:CS:42:ASN:HD21  | 2.17                     | 0.52              |
| 23:DB:288:U:O2'    | 23:DB:289:G:H5'    | 2.08                     | 0.52              |
| 23:DB:448:U:H3'    | 27:DE:79:ARG:NE    | 2.23                     | 0.52              |
| 23:DB:533:G:H5'    | 38:DQ:23:TYR:HD1   | 1.73                     | 0.52              |
| 23:DB:1099:G:N7    | 52:DI:3:LYS:HD3    | 2.25                     | 0.52              |
| 23:DB:2280:G:O6    | 43:DW:10:ARG:NH2   | 2.41                     | 0.52              |
| 23:DB:2774:C:H2'   | 23:DB:2775:G:O4'   | 2.09                     | 0.52              |
| 23:DB:2794:C:H2'   | 23:DB:2795:C:C6    | 2.44                     | 0.52              |
| 23:DB:2898:U:H2'   | 23:DB:2899:A:C8    | 2.45                     | 0.52              |
| 24:DV:9:ARG:HE     | 24:DV:20:LEU:HD11  | 1.74                     | 0.52              |
| 25:DC:226:PRO:HG3  | 25:DC:232:GLY:O    | 2.10                     | 0.52              |
| 28:DF:9:ASP:O      | 28:DF:10:GLU:HB2   | 2.08                     | 0.52              |
| 28:DF:18:GLU:C     | 28:DF:20:ASN:N     | 2.66                     | 0.52              |
| 35:DN:4:ARG:CZ     | 35:DN:4:ARG:N      | 2.73                     | 0.52              |
| 35:DN:10:LEU:HG    | 35:DN:11:ASN:N     | 2.24                     | 0.52              |
| 38:DQ:52:ARG:HG2   | 38:DQ:53:LYS:NZ    | 2.24                     | 0.52              |
| 48:D1:20:TYR:O     | 48:D1:21:THR:HB    | 2.09                     | 0.52              |
| 48:D1:46:VAL:HG22  | 48:D1:47:ILE:N     | 2.24                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:D2:12:ARG:HH21  | 49:D2:16:HIS:CB    | 2.22                     | 0.52              |
| 51:D4:2:LYS:HB2    | 51:D4:2:LYS:HZ2    | 1.73                     | 0.52              |
| 1:AA:33:A:H2'      | 1:AA:34:C:C6       | 2.45                     | 0.52              |
| 1:AA:246:A:C2      | 1:AA:282:A:C5      | 2.98                     | 0.52              |
| 1:AA:303:A:H2'     | 1:AA:304:U:O4'     | 2.10                     | 0.52              |
| 1:AA:520:A:OP2     | 11:AL:47:ALA:HB1   | 2.09                     | 0.52              |
| 1:AA:528:C:H41     | 11:AL:45:ASN:CG    | 2.17                     | 0.52              |
| 1:AA:860:A:H2'     | 1:AA:861:G:O4'     | 2.09                     | 0.52              |
| 1:AA:1170:A:H8     | 1:AA:1170:A:O5'    | 1.92                     | 0.52              |
| 1:AA:1256:A:O2'    | 1:AA:1257:A:H5''   | 2.09                     | 0.52              |
| 4:AE:150:GLU:C     | 4:AE:152:VAL:H     | 2.17                     | 0.52              |
| 8:AI:24:ASN:CA     | 8:AI:26:LYS:HZ2    | 2.22                     | 0.52              |
| 8:AI:29:ILE:HD11   | 8:AI:37:TYR:HB3    | 1.92                     | 0.52              |
| 17:AR:20:ILE:HG23  | 17:AR:53:GLN:NE2   | 2.25                     | 0.52              |
| 20:AB:20:ARG:HG3   | 20:AB:20:ARG:HH11  | 1.73                     | 0.52              |
| 20:AB:36:LYS:HE3   | 20:AB:36:LYS:H     | 1.71                     | 0.52              |
| 20:AB:71:THR:HB    | 20:AB:167:HIS:CD2  | 2.44                     | 0.52              |
| 20:AB:95:TRP:HH2   | 20:AB:100:LEU:HB2  | 1.74                     | 0.52              |
| 20:AB:172:ILE:HG22 | 20:AB:176:ASN:ND2  | 2.25                     | 0.52              |
| 23:BB:142:A:C4     | 41:BT:2:ILE:HD12   | 2.44                     | 0.52              |
| 23:BB:464:U:H2'    | 23:BB:465:G:O4'    | 2.10                     | 0.52              |
| 23:BB:576:U:H2'    | 23:BB:577:G:C8     | 2.45                     | 0.52              |
| 23:BB:1000:A:H2'   | 23:BB:1001:A:C8    | 2.45                     | 0.52              |
| 23:BB:1506:U:H2'   | 23:BB:1507:C:C6    | 2.45                     | 0.52              |
| 23:BB:1658:C:OP1   | 26:BD:136:ASN:HA   | 2.10                     | 0.52              |
| 23:BB:1973:G:H2'   | 23:BB:1974:C:H6    | 1.75                     | 0.52              |
| 23:BB:2014:A:OP1   | 40:BS:95:ARG:HB2   | 2.09                     | 0.52              |
| 23:BB:2137:U:H6    | 23:BB:2137:U:O5'   | 1.93                     | 0.52              |
| 23:BB:2298:A:H2'   | 23:BB:2299:U:O4'   | 2.10                     | 0.52              |
| 24:BV:42:LEU:HD12  | 24:BV:47:VAL:HG11  | 1.90                     | 0.52              |
| 25:BC:20:ASN:HB2   | 25:BC:203:VAL:CG1  | 2.39                     | 0.52              |
| 25:BC:29:PHE:CD1   | 25:BC:29:PHE:C     | 2.87                     | 0.52              |
| 25:BC:112:GLY:O    | 25:BC:113:ASP:HB2  | 2.08                     | 0.52              |
| 26:BD:165:MET:HG3  | 26:BD:166:GLY:H    | 1.74                     | 0.52              |
| 27:BE:141:MET:HG3  | 27:BE:143:LEU:HB2  | 1.91                     | 0.52              |
| 30:BH:5:LEU:C      | 30:BH:7:ASP:H      | 2.18                     | 0.52              |
| 31:BJ:7:LYS:C      | 31:BJ:9:GLU:H      | 2.17                     | 0.52              |
| 33:BL:63:LYS:HD3   | 33:BL:63:LYS:O     | 2.10                     | 0.52              |
| 33:BL:116:VAL:HG11 | 33:BL:134:ALA:O    | 2.08                     | 0.52              |
| 33:BL:126:ARG:HD3  | 33:BL:126:ARG:C    | 2.34                     | 0.52              |
| 34:BM:33:LEU:HD13  | 34:BM:124:LEU:HD11 | 1.92                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:BN:75:ILE:HD13 | 35:BN:75:ILE:C    | 2.35                     | 0.52              |
| 37:BP:93:LYS:HB2  | 37:BP:96:LEU:HA   | 1.91                     | 0.52              |
| 42:BU:11:ILE:HB   | 42:BU:69:VAL:CG1  | 2.40                     | 0.52              |
| 42:BU:60:LYS:HG3  | 42:BU:61:GLU:N    | 2.24                     | 0.52              |
| 43:BW:66:VAL:HG13 | 43:BW:67:LYS:HG3  | 1.90                     | 0.52              |
| 1:CA:777:A:H2'    | 1:CA:778:G:C8     | 2.43                     | 0.52              |
| 1:CA:1009:U:H2'   | 1:CA:1010:U:C6    | 2.44                     | 0.52              |
| 1:CA:1070:U:H2'   | 1:CA:1071:C:H6    | 1.74                     | 0.52              |
| 1:CA:1137:C:H1'   | 1:CA:1138:G:C2    | 2.44                     | 0.52              |
| 7:CH:111:THR:H    | 7:CH:114:ALA:HB3  | 1.74                     | 0.52              |
| 11:CL:6:LEU:HB3   | 16:CQ:33:TYR:OH   | 2.09                     | 0.52              |
| 11:CL:8:ARG:O     | 11:CL:10:PRO:HD3  | 2.08                     | 0.52              |
| 22:DA:52:A:H2'    | 22:DA:53:A:H8     | 1.74                     | 0.52              |
| 23:DB:110:G:O2'   | 23:DB:111:A:H5'   | 2.09                     | 0.52              |
| 23:DB:1099:G:O5'  | 52:DI:3:LYS:CA    | 2.57                     | 0.52              |
| 23:DB:1341:G:H1'  | 41:DT:59:ASN:HB3  | 1.90                     | 0.52              |
| 23:DB:1857:G:H2'  | 23:DB:1884:G:N2   | 2.24                     | 0.52              |
| 23:DB:2364:C:H2'  | 23:DB:2365:G:O4'  | 2.10                     | 0.52              |
| 23:DB:2882:A:OP1  | 35:DN:96:ARG:HD2  | 2.10                     | 0.52              |
| 25:DC:172:THR:O   | 25:DC:173:LEU:CB  | 2.56                     | 0.52              |
| 26:DD:122:VAL:HA  | 26:DD:128:ARG:CD  | 2.39                     | 0.52              |
| 28:DF:55:ASP:O    | 28:DF:59:ILE:HB   | 2.10                     | 0.52              |
| 32:DK:15:GLY:HA3  | 32:DK:52:VAL:HB   | 1.92                     | 0.52              |
| 33:DL:59:ARG:HH21 | 50:D3:5:THR:HB    | 1.75                     | 0.52              |
| 33:DL:89:VAL:HG21 | 33:DL:123:ARG:CZ  | 2.39                     | 0.52              |
| 35:DN:123:GLU:CG  | 35:DN:124:ALA:H   | 2.23                     | 0.52              |
| 36:DO:27:VAL:HG13 | 36:DO:40:ILE:HD11 | 1.91                     | 0.52              |
| 37:DP:25:VAL:O    | 37:DP:47:ILE:HB   | 2.10                     | 0.52              |
| 38:DQ:82:LEU:CD1  | 38:DQ:112:ALA:HB2 | 2.39                     | 0.52              |
| 39:DR:78:ARG:HD2  | 39:DR:88:GLY:O    | 2.09                     | 0.52              |
| 40:DS:28:LYS:HB3  | 40:DS:31:GLN:HB2  | 1.92                     | 0.52              |
| 42:DU:82:VAL:HG21 | 42:DU:95:PHE:O    | 2.09                     | 0.52              |
| 43:DW:38:ARG:HE   | 43:DW:40:ARG:HA   | 1.75                     | 0.52              |
| 52:DI:73:PRO:CG   | 52:DI:78:LEU:HD21 | 2.39                     | 0.52              |
| 1:AA:78:A:H8      | 1:AA:78:A:O5'     | 1.93                     | 0.52              |
| 1:AA:663:A:O2'    | 1:AA:664:G:H5'    | 2.09                     | 0.52              |
| 1:AA:986:U:H1'    | 18:AS:53:GLY:O    | 2.10                     | 0.52              |
| 1:AA:1414:U:H2'   | 1:AA:1415:G:H8    | 1.74                     | 0.52              |
| 3:AD:159:GLU:HG3  | 3:AD:160:LEU:HD13 | 1.91                     | 0.52              |
| 4:AE:40:ASP:C     | 4:AE:42:ASN:H     | 2.17                     | 0.52              |
| 6:AG:62:GLU:O     | 6:AG:66:GLU:HG3   | 2.10                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:AN:65:GLN:HA   | 13:AN:65:GLN:HE21 | 1.74                     | 0.52              |
| 23:BB:65:U:H2'    | 23:BB:66:C:C6     | 2.44                     | 0.52              |
| 23:BB:170:U:O2'   | 23:BB:171:U:H5'   | 2.09                     | 0.52              |
| 23:BB:540:C:O2'   | 23:BB:541:A:H5'   | 2.10                     | 0.52              |
| 23:BB:554:U:H2'   | 23:BB:555:G:O4'   | 2.10                     | 0.52              |
| 23:BB:580:U:H2'   | 23:BB:581:C:H6    | 1.70                     | 0.52              |
| 23:BB:991:C:H2'   | 23:BB:992:C:H6    | 1.74                     | 0.52              |
| 23:BB:1076:C:H4'  | 52:BI:94:LYS:HZ2  | 1.74                     | 0.52              |
| 23:BB:1374:G:H2'  | 23:BB:1375:U:C6   | 2.45                     | 0.52              |
| 23:BB:1656:C:H2'  | 23:BB:1657:U:H6   | 1.74                     | 0.52              |
| 23:BB:2405:G:H1'  | 23:BB:2412:A:H61  | 1.75                     | 0.52              |
| 23:BB:2742:G:OP1  | 51:B4:36:ARG:NE   | 2.43                     | 0.52              |
| 24:BV:21:ARG:HE   | 24:BV:87:GLN:CB   | 2.23                     | 0.52              |
| 24:BV:80:HIS:HB3  | 24:BV:83:LYS:O    | 2.09                     | 0.52              |
| 25:BC:24:HIS:CB   | 25:BC:27:LYS:HE3  | 2.39                     | 0.52              |
| 25:BC:124:LYS:HB2 | 25:BC:125:PRO:HD2 | 1.91                     | 0.52              |
| 26:BD:4:LEU:H     | 26:BD:49:GLN:NE2  | 2.08                     | 0.52              |
| 26:BD:101:PHE:O   | 26:BD:102:ALA:HB3 | 2.10                     | 0.52              |
| 33:BL:29:LYS:CD   | 33:BL:30:THR:H    | 2.18                     | 0.52              |
| 34:BM:1:MET:HA    | 34:BM:65:ILE:HG12 | 1.90                     | 0.52              |
| 36:BO:19:GLN:HA   | 43:BW:76:ARG:NH2  | 2.25                     | 0.52              |
| 36:BO:30:ARG:HH11 | 36:BO:30:ARG:HG2  | 1.75                     | 0.52              |
| 36:BO:55:GLU:HB2  | 36:BO:60:GLU:O    | 2.10                     | 0.52              |
| 38:BQ:57:ARG:HA   | 38:BQ:60:TRP:CE3  | 2.43                     | 0.52              |
| 39:BR:78:ARG:CB   | 39:BR:87:GLN:HA   | 2.31                     | 0.52              |
| 43:BW:22:VAL:HG12 | 43:BW:23:LYS:N    | 2.25                     | 0.52              |
| 46:BZ:64:PHE:CA   | 46:BZ:67:PRO:HD2  | 2.39                     | 0.52              |
| 49:B2:8:SER:OG    | 49:B2:11:LYS:HD3  | 2.09                     | 0.52              |
| 1:CA:33:A:H2'     | 1:CA:34:C:C6      | 2.45                     | 0.52              |
| 1:CA:82:G:H2'     | 1:CA:83:C:O4'     | 2.09                     | 0.52              |
| 1:CA:474:G:H2'    | 1:CA:475:C:H6     | 1.73                     | 0.52              |
| 1:CA:711:G:O2'    | 1:CA:712:A:H5'    | 2.10                     | 0.52              |
| 1:CA:730:G:O2'    | 1:CA:766:A:H5'    | 2.08                     | 0.52              |
| 1:CA:939:G:H5''   | 6:CG:101:ARG:CZ   | 2.40                     | 0.52              |
| 1:CA:1074:G:H2'   | 1:CA:1075:U:H6    | 1.74                     | 0.52              |
| 1:CA:1149:C:O2'   | 1:CA:1150:A:H5'   | 2.09                     | 0.52              |
| 1:CA:1307:U:H2'   | 1:CA:1308:U:C6    | 2.45                     | 0.52              |
| 1:CA:1351:U:O2'   | 1:CA:1352:C:H5'   | 2.10                     | 0.52              |
| 2:CC:149:LYS:HG3  | 2:CC:166:TRP:NE1  | 2.24                     | 0.52              |
| 3:CD:18:LEU:HD12  | 3:CD:63:ILE:HB    | 1.91                     | 0.52              |
| 5:CF:92:THR:O     | 5:CF:93:LYS:HB2   | 2.09                     | 0.52              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:CJ:55:PRO:HA    | 13:CN:80:ARG:NH2  | 2.24                     | 0.52              |
| 14:CO:62:ARG:NH1  | 14:CO:86:LEU:HD21 | 2.25                     | 0.52              |
| 23:DB:137:U:C2'   | 23:DB:138:U:H5'   | 2.39                     | 0.52              |
| 23:DB:448:U:O4'   | 23:DB:448:U:O2    | 2.27                     | 0.52              |
| 23:DB:589:U:H2'   | 23:DB:590:A:H8    | 1.72                     | 0.52              |
| 23:DB:737:C:O2'   | 23:DB:738:G:H5'   | 2.09                     | 0.52              |
| 23:DB:931:U:H3    | 23:DB:1166:G:N2   | 2.07                     | 0.52              |
| 23:DB:1050:A:H2'  | 23:DB:1051:G:O4'  | 2.09                     | 0.52              |
| 23:DB:1133:A:H2   | 23:DB:2038:G:H21  | 1.58                     | 0.52              |
| 23:DB:1252:G:H21  | 38:DQ:32:ARG:NE   | 2.07                     | 0.52              |
| 23:DB:1309:G:H5'  | 49:D2:7:PRO:HB2   | 1.90                     | 0.52              |
| 23:DB:1506:U:H2'  | 23:DB:1507:C:C6   | 2.45                     | 0.52              |
| 23:DB:1739:A:H2'  | 23:DB:1740:G:O4'  | 2.10                     | 0.52              |
| 23:DB:1986:C:O2'  | 23:DB:1987:A:H5'  | 2.10                     | 0.52              |
| 23:DB:2083:G:H2'  | 23:DB:2084:C:H6   | 1.75                     | 0.52              |
| 23:DB:2719:G:H4'  | 23:DB:2846:G:O3'  | 2.09                     | 0.52              |
| 25:DC:86:ARG:C    | 25:DC:155:ARG:NH1 | 2.68                     | 0.52              |
| 26:DD:31:ALA:HA   | 26:DD:51:THR:CA   | 2.34                     | 0.52              |
| 26:DD:123:LYS:HE3 | 26:DD:165:MET:HE2 | 1.92                     | 0.52              |
| 26:DD:139:SER:O   | 26:DD:141:ARG:N   | 2.42                     | 0.52              |
| 27:DE:46:GLN:NE2  | 27:DE:87:ALA:N    | 2.58                     | 0.52              |
| 29:DG:41:GLU:HB2  | 29:DG:52:GLY:HA3  | 1.92                     | 0.52              |
| 31:DJ:10:THR:O    | 31:DJ:11:VAL:HB   | 2.08                     | 0.52              |
| 31:DJ:49:ASP:O    | 31:DJ:50:THR:HB   | 2.09                     | 0.52              |
| 31:DJ:120:ARG:HB3 | 31:DJ:121:LYS:HZ1 | 1.74                     | 0.52              |
| 32:DK:19:VAL:C    | 32:DK:41:ILE:HD11 | 2.34                     | 0.52              |
| 33:DL:19:LEU:HD22 | 33:DL:19:LEU:N    | 2.24                     | 0.52              |
| 34:DM:118:LYS:HB2 | 34:DM:118:LYS:HZ2 | 1.74                     | 0.52              |
| 36:DO:15:ARG:HH22 | 43:DW:76:ARG:CG   | 2.22                     | 0.52              |
| 38:DQ:47:ARG:HH22 | 38:DQ:50:ARG:HB2  | 1.75                     | 0.52              |
| 39:DR:4:VAL:HG11  | 39:DR:46:GLU:OE2  | 2.10                     | 0.52              |
| 39:DR:6:GLN:CG    | 39:DR:7:SER:H     | 2.18                     | 0.52              |
| 40:DS:7:HIS:CD2   | 40:DS:46:LEU:HD13 | 2.44                     | 0.52              |
| 43:DW:36:ILE:HD12 | 43:DW:37:VAL:H    | 1.73                     | 0.52              |
| 43:DW:44:PHE:HB3  | 43:DW:77:LYS:O    | 2.09                     | 0.52              |
| 51:D4:18:LYS:HE2  | 51:D4:19:ARG:H    | 1.68                     | 0.52              |
| 1:AA:462:G:H2'    | 1:AA:463:U:C6     | 2.44                     | 0.52              |
| 1:AA:764:C:C2'    | 1:AA:765:G:H5'    | 2.39                     | 0.52              |
| 1:AA:894:G:O2'    | 1:AA:895:G:H5'    | 2.10                     | 0.52              |
| 1:AA:924:C:O2'    | 1:AA:925:G:H5'    | 2.08                     | 0.52              |
| 1:AA:1510:C:H2'   | 1:AA:1511:G:C8    | 2.44                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:AE:35:LEU:HD11   | 4:AE:136:VAL:HG11  | 1.92                     | 0.52              |
| 16:AQ:16:MET:CB    | 16:AQ:19:SER:HB2   | 2.39                     | 0.52              |
| 21:AU:13:VAL:O     | 21:AU:14:ALA:HB2   | 2.09                     | 0.52              |
| 23:BB:27:G:H1'     | 23:BB:513:A:H61    | 1.74                     | 0.52              |
| 23:BB:107:G:H21    | 23:BB:346:A:H62    | 1.57                     | 0.52              |
| 23:BB:656:G:H2'    | 23:BB:657:U:C6     | 2.45                     | 0.52              |
| 23:BB:920:A:H2'    | 23:BB:921:C:H6     | 1.75                     | 0.52              |
| 23:BB:1149:G:H2'   | 23:BB:1150:C:H6    | 1.74                     | 0.52              |
| 23:BB:1274:A:N3    | 23:BB:1297:C:H1'   | 2.25                     | 0.52              |
| 23:BB:1341:G:H2'   | 23:BB:1397:U:O2'   | 2.09                     | 0.52              |
| 23:BB:1717:A:H2'   | 23:BB:1718:G:O4'   | 2.10                     | 0.52              |
| 23:BB:2070:A:H2'   | 23:BB:2071:A:H8    | 1.74                     | 0.52              |
| 24:BV:5:ASN:HA     | 24:BV:64:VAL:HB    | 1.92                     | 0.52              |
| 25:BC:61:TYR:CZ    | 25:BC:63:ILE:HD11  | 2.45                     | 0.52              |
| 26:BD:34:VAL:HG23  | 26:BD:93:GLY:O     | 2.09                     | 0.52              |
| 26:BD:206:ALA:C    | 26:BD:208:LYS:H    | 2.17                     | 0.52              |
| 28:BF:103:ILE:HA   | 28:BF:107:VAL:HG21 | 1.90                     | 0.52              |
| 32:BK:63:VAL:HG12  | 32:BK:103:VAL:HA   | 1.92                     | 0.52              |
| 32:BK:118:LEU:HD12 | 32:BK:118:LEU:N    | 2.24                     | 0.52              |
| 34:BM:65:ILE:HG22  | 34:BM:101:VAL:HG12 | 1.92                     | 0.52              |
| 38:BQ:33:VAL:O     | 38:BQ:34:ALA:C     | 2.53                     | 0.52              |
| 40:BS:28:LYS:HB3   | 40:BS:71:VAL:CG2   | 2.40                     | 0.52              |
| 43:BW:65:LYS:O     | 43:BW:66:VAL:HB    | 2.08                     | 0.52              |
| 44:BX:47:ARG:HG2   | 44:BX:47:ARG:O     | 2.10                     | 0.52              |
| 45:BY:3:THR:HA     | 45:BY:47:ILE:CD1   | 2.39                     | 0.52              |
| 45:BY:9:THR:CB     | 45:BY:54:VAL:HA    | 2.34                     | 0.52              |
| 51:B4:24:ARG:HG2   | 51:B4:26:ILE:H     | 1.74                     | 0.52              |
| 52:BI:32:VAL:HG22  | 52:BI:60:VAL:CG2   | 2.40                     | 0.52              |
| 1:CA:303:A:H2'     | 1:CA:304:U:O4'     | 2.10                     | 0.52              |
| 1:CA:769:G:H4'     | 1:CA:1513:A:H4'    | 1.92                     | 0.52              |
| 1:CA:1213:A:O2'    | 1:CA:1214:C:H5''   | 2.10                     | 0.52              |
| 1:CA:1317:C:H2'    | 1:CA:1318:A:O4'    | 2.10                     | 0.52              |
| 6:CG:49:LEU:O      | 6:CG:49:LEU:HD23   | 2.09                     | 0.52              |
| 12:CM:100:ARG:HB2  | 12:CM:102:LYS:HG2  | 1.91                     | 0.52              |
| 15:CP:22:ALA:CB    | 15:CP:32:PHE:HA    | 2.40                     | 0.52              |
| 20:CB:44:LYS:O     | 20:CB:47:PRO:HD2   | 2.10                     | 0.52              |
| 21:CU:8:ASN:HB2    | 21:CU:9:GLU:CD     | 2.34                     | 0.52              |
| 21:CU:48:LYS:HD2   | 21:CU:48:LYS:C     | 2.35                     | 0.52              |
| 23:DB:419:U:H2'    | 23:DB:420:C:H6     | 1.75                     | 0.52              |
| 23:DB:600:G:H2'    | 23:DB:601:C:C6     | 2.44                     | 0.52              |
| 23:DB:686:U:H1'    | 49:D2:5:PHE:O      | 2.10                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:1386:C:H2'   | 23:DB:1387:A:H8    | 1.74                     | 0.52              |
| 23:DB:1745:A:O2'   | 23:DB:1746:A:H5'   | 2.09                     | 0.52              |
| 23:DB:1818:U:H5''  | 25:DC:155:ARG:HG2  | 1.92                     | 0.52              |
| 23:DB:1845:G:O2'   | 23:DB:1846:G:H5'   | 2.10                     | 0.52              |
| 23:DB:1957:C:H2'   | 23:DB:1958:C:H6    | 1.74                     | 0.52              |
| 23:DB:2250:G:H21   | 23:DB:2496:C:C4'   | 2.22                     | 0.52              |
| 23:DB:2316:G:O2'   | 23:DB:2317:A:H5'   | 2.10                     | 0.52              |
| 55:DB:3322:HOH:O   | 27:DE:63:LYS:HE2   | 2.09                     | 0.52              |
| 25:DC:179:GLU:OE2  | 25:DC:267:VAL:HG23 | 2.10                     | 0.52              |
| 25:DC:231:HIS:ND1  | 25:DC:242:HIS:ND1  | 2.56                     | 0.52              |
| 26:DD:4:LEU:CD1    | 26:DD:79:LEU:HD22  | 2.40                     | 0.52              |
| 26:DD:129:THR:O    | 26:DD:140:HIS:HA   | 2.10                     | 0.52              |
| 27:DE:21:ARG:HD3   | 27:DE:25:GLU:CB    | 2.40                     | 0.52              |
| 27:DE:147:LEU:HB2  | 27:DE:183:PHE:CD1  | 2.45                     | 0.52              |
| 31:DJ:100:VAL:O    | 31:DJ:101:ILE:HB   | 2.10                     | 0.52              |
| 32:DK:20:MET:C     | 32:DK:41:ILE:HD12  | 2.34                     | 0.52              |
| 33:DL:34:GLY:CA    | 39:DR:85:LYS:HE2   | 2.40                     | 0.52              |
| 33:DL:118:THR:C    | 33:DL:120:VAL:N    | 2.64                     | 0.52              |
| 35:DN:14:SER:HA    | 35:DN:17:ARG:NH2   | 2.24                     | 0.52              |
| 37:DP:52:ARG:O     | 37:DP:60:VAL:HG21  | 2.09                     | 0.52              |
| 38:DQ:46:TYR:HA    | 39:DR:77:PHE:CD2   | 2.43                     | 0.52              |
| 41:DT:86:THR:O     | 41:DT:87:LEU:HB2   | 2.08                     | 0.52              |
| 46:DZ:5:ILE:HG13   | 46:DZ:51:VAL:CG1   | 2.38                     | 0.52              |
| 50:D3:46:LYS:HD2   | 50:D3:47:ALA:H     | 1.72                     | 0.52              |
| 52:DI:105:LEU:HD11 | 52:DI:139:VAL:CG2  | 2.36                     | 0.52              |
| 1:AA:60:A:O2'      | 1:AA:61:G:P        | 2.66                     | 0.52              |
| 1:AA:217:C:O2'     | 1:AA:218:U:H5'     | 2.10                     | 0.52              |
| 1:AA:541:G:H2'     | 1:AA:542:G:H8      | 1.75                     | 0.52              |
| 1:AA:677:U:H2'     | 1:AA:678:U:C6      | 2.44                     | 0.52              |
| 1:AA:1243:C:H2'    | 1:AA:1244:G:H8     | 1.75                     | 0.52              |
| 1:AA:1518:A:H2'    | 1:AA:1519:A:C8     | 2.45                     | 0.52              |
| 12:AM:53:ASP:HA    | 12:AM:56:ARG:CD    | 2.40                     | 0.52              |
| 22:BA:32:U:H2'     | 22:BA:33:G:O4'     | 2.09                     | 0.52              |
| 23:BB:52:A:C5      | 23:BB:118:A:C2     | 2.98                     | 0.52              |
| 23:BB:397:U:H2'    | 23:BB:398:C:C6     | 2.45                     | 0.52              |
| 23:BB:570:G:H2'    | 23:BB:2030:A:N7    | 2.24                     | 0.52              |
| 23:BB:807:U:O2'    | 23:BB:808:G:H5'    | 2.10                     | 0.52              |
| 23:BB:1256:G:H21   | 27:BE:77:ILE:HG23  | 1.75                     | 0.52              |
| 23:BB:1545:A:H2'   | 23:BB:1546:G:O4'   | 2.09                     | 0.52              |
| 23:BB:1791:A:H5'   | 25:BC:207:ALA:HA   | 1.91                     | 0.52              |
| 23:BB:1957:C:H2'   | 23:BB:1958:C:H6    | 1.74                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BB:2189:U:H2'  | 23:BB:2190:G:H8   | 1.74                     | 0.52              |
| 23:BB:2229:U:H2'  | 23:BB:2230:G:C8   | 2.45                     | 0.52              |
| 25:BC:141:HIS:HD2 | 25:BC:193:GLU:H   | 1.57                     | 0.52              |
| 25:BC:230:PRO:O   | 25:BC:231:HIS:HB3 | 2.09                     | 0.52              |
| 26:BD:77:ARG:HG2  | 26:BD:78:GLY:N    | 2.23                     | 0.52              |
| 26:BD:115:GLY:HA3 | 26:BD:166:GLY:CA  | 2.39                     | 0.52              |
| 27:BE:165:HIS:C   | 27:BE:166:LYS:HG3 | 2.35                     | 0.52              |
| 31:BJ:75:TYR:CD2  | 31:BJ:75:TYR:N    | 2.78                     | 0.52              |
| 37:BP:61:ARG:CZ   | 37:BP:61:ARG:HB2  | 2.40                     | 0.52              |
| 41:BT:93:LEU:HD22 | 41:BT:93:LEU:N    | 2.23                     | 0.52              |
| 42:BU:38:ILE:O    | 42:BU:39:ASN:HB2  | 2.08                     | 0.52              |
| 52:BI:76:ALA:O    | 52:BI:80:LYS:HG3  | 2.10                     | 0.52              |
| 1:CA:287:U:O2'    | 1:CA:288:A:H5'    | 2.08                     | 0.52              |
| 1:CA:323:U:H2'    | 1:CA:324:G:O4'    | 2.10                     | 0.52              |
| 1:CA:1226:C:H5''  | 12:CM:101:THR:O   | 2.10                     | 0.52              |
| 4:CE:149:PRO:HG2  | 4:CE:150:GLU:OE2  | 2.09                     | 0.52              |
| 6:CG:55:LYS:HB3   | 6:CG:59:GLU:CD    | 2.35                     | 0.52              |
| 9:CJ:9:ARG:CB     | 9:CJ:99:GLN:HG3   | 2.39                     | 0.52              |
| 11:CL:97:VAL:O    | 11:CL:97:VAL:HG23 | 2.09                     | 0.52              |
| 12:CM:68:LEU:HD22 | 12:CM:69:ARG:NH1  | 2.25                     | 0.52              |
| 23:DB:807:U:O2'   | 23:DB:808:G:H5'   | 2.10                     | 0.52              |
| 23:DB:1516:G:O2'  | 23:DB:1517:G:H5'  | 2.10                     | 0.52              |
| 23:DB:2135:A:C2   | 23:DB:2136:G:C8   | 2.98                     | 0.52              |
| 23:DB:2688:G:H1'  | 23:DB:2721:A:H61  | 1.74                     | 0.52              |
| 31:DJ:41:LYS:CD   | 31:DJ:44:TYR:HB3  | 2.39                     | 0.52              |
| 33:DL:62:PRO:HB3  | 50:D3:12:ARG:CD   | 2.40                     | 0.52              |
| 33:DL:123:ARG:CA  | 33:DL:142:ILE:HA  | 2.39                     | 0.52              |
| 34:DM:41:LEU:CG   | 34:DM:46:ILE:HD11 | 2.40                     | 0.52              |
| 35:DN:63:ARG:HA   | 35:DN:80:PHE:CZ   | 2.45                     | 0.52              |
| 37:DP:50:ARG:HG3  | 37:DP:99:LEU:H    | 1.75                     | 0.52              |
| 39:DR:44:GLY:H    | 39:DR:53:PHE:HE2  | 1.57                     | 0.52              |
| 39:DR:76:LYS:HB3  | 39:DR:90:ARG:CB   | 2.40                     | 0.52              |
| 39:DR:78:ARG:O    | 39:DR:79:ARG:HB2  | 2.09                     | 0.52              |
| 41:DT:38:ALA:O    | 41:DT:42:GLU:HB3  | 2.10                     | 0.52              |
| 41:DT:65:GLY:HA3  | 41:DT:76:ARG:NH2  | 2.25                     | 0.52              |
| 43:DW:60:ALA:CB   | 43:DW:80:SER:HA   | 2.37                     | 0.52              |
| 44:DX:6:LEU:HD22  | 44:DX:56:LEU:HD12 | 1.92                     | 0.52              |
| 46:DZ:36:VAL:O    | 46:DZ:36:VAL:HG23 | 2.10                     | 0.52              |
| 50:D3:33:THR:HG22 | 50:D3:40:LYS:HD2  | 1.91                     | 0.52              |
| 50:D3:40:LYS:O    | 50:D3:43:LEU:HD13 | 2.10                     | 0.52              |
| 52:DI:116:MET:HE1 | 52:DI:128:ILE:CG1 | 2.40                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:442:G:H2'     | 1:AA:443:C:C6      | 2.45                     | 0.52              |
| 1:AA:1410:A:H2'    | 1:AA:1411:C:C6     | 2.45                     | 0.52              |
| 2:AC:30:ASP:O      | 2:AC:33:ASP:HB3    | 2.09                     | 0.52              |
| 2:AC:61:LYS:O      | 2:AC:96:VAL:HB     | 2.09                     | 0.52              |
| 2:AC:87:ARG:HG3    | 2:AC:100:ILE:CG2   | 2.38                     | 0.52              |
| 2:AC:154:GLY:HA2   | 2:AC:163:ARG:H     | 1.73                     | 0.52              |
| 3:AD:99:ASN:ND2    | 3:AD:110:ARG:HE    | 2.08                     | 0.52              |
| 6:AG:41:ILE:HG13   | 6:AG:116:ALA:HA    | 1.91                     | 0.52              |
| 7:AH:12:ARG:NH1    | 7:AH:26:MET:HB2    | 2.24                     | 0.52              |
| 17:AR:70:THR:HG23  | 17:AR:71:ASP:H     | 1.75                     | 0.52              |
| 20:AB:131:LYS:HE3  | 20:AB:135:MET:HE2  | 1.92                     | 0.52              |
| 23:BB:396:G:H5'    | 46:BZ:9:TYR:CB     | 2.34                     | 0.52              |
| 23:BB:416:U:H2'    | 23:BB:417:C:H6     | 1.75                     | 0.52              |
| 23:BB:526:A:N6     | 23:BB:2626:C:C4'   | 2.73                     | 0.52              |
| 23:BB:558:U:P      | 31:BJ:113:PRO:HG2  | 2.50                     | 0.52              |
| 23:BB:753:A:H2'    | 23:BB:754:U:C6     | 2.45                     | 0.52              |
| 23:BB:773:U:H5'    | 23:BB:774:G:OP2    | 2.10                     | 0.52              |
| 23:BB:973:A:H8     | 23:BB:973:A:OP1    | 1.92                     | 0.52              |
| 23:BB:978:G:H2'    | 23:BB:979:A:H8     | 1.75                     | 0.52              |
| 23:BB:1213:A:C6    | 23:BB:1237:A:H1'   | 2.45                     | 0.52              |
| 23:BB:1845:G:O2'   | 23:BB:1846:G:H5'   | 2.10                     | 0.52              |
| 23:BB:2077:A:H2'   | 23:BB:2078:C:H6    | 1.72                     | 0.52              |
| 23:BB:2186:G:H2'   | 23:BB:2187:U:O4'   | 2.10                     | 0.52              |
| 23:BB:2354:C:O3'   | 43:BW:30:VAL:HG13  | 2.10                     | 0.52              |
| 23:BB:2373:G:H2'   | 23:BB:2374:C:C6    | 2.45                     | 0.52              |
| 24:BV:66:ASP:C     | 24:BV:68:LYS:H     | 2.18                     | 0.52              |
| 24:BV:82:TYR:N     | 24:BV:82:TYR:HD2   | 2.08                     | 0.52              |
| 25:BC:51:ARG:O     | 25:BC:51:ARG:CD    | 2.58                     | 0.52              |
| 25:BC:140:VAL:HG11 | 25:BC:163:ILE:HD11 | 1.92                     | 0.52              |
| 28:BF:135:ILE:HB   | 28:BF:142:TYR:CE1  | 2.45                     | 0.52              |
| 28:BF:136:ILE:HD12 | 28:BF:136:ILE:N    | 2.25                     | 0.52              |
| 31:BJ:1:MET:SD     | 39:BR:14:VAL:HG21  | 2.50                     | 0.52              |
| 31:BJ:10:THR:HG22  | 31:BJ:50:THR:HA    | 1.90                     | 0.52              |
| 34:BM:67:VAL:HB    | 34:BM:100:LYS:CD   | 2.40                     | 0.52              |
| 35:BN:122:ALA:HA   | 47:B0:49:ARG:NH1   | 2.25                     | 0.52              |
| 37:BP:63:ILE:HD12  | 37:BP:63:ILE:N     | 2.24                     | 0.52              |
| 40:BS:11:ARG:HA    | 40:BS:100:THR:HG22 | 1.92                     | 0.52              |
| 41:BT:86:THR:C     | 41:BT:87:LEU:HD22  | 2.35                     | 0.52              |
| 42:BU:73:ASN:HB2   | 42:BU:96:LYS:HZ2   | 1.75                     | 0.52              |
| 1:CA:394:G:H2'     | 1:CA:395:C:C6      | 2.45                     | 0.52              |
| 1:CA:537:G:H2'     | 1:CA:538:G:C8      | 2.45                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1354:U:H2'   | 1:CA:1355:G:C8    | 2.44                     | 0.52              |
| 1:CA:1355:G:O2'   | 1:CA:1356:G:H5'   | 2.10                     | 0.52              |
| 2:CC:156:LEU:HD12 | 2:CC:163:ARG:HG3  | 1.91                     | 0.52              |
| 6:CG:96:ASN:O     | 6:CG:100:MET:HG2  | 2.10                     | 0.52              |
| 8:CI:9:GLY:HA2    | 8:CI:80:HIS:HB3   | 1.92                     | 0.52              |
| 8:CI:40:ARG:HA    | 8:CI:44:ARG:CZ    | 2.40                     | 0.52              |
| 10:CK:85:VAL:CG2  | 10:CK:92:ARG:HH12 | 2.22                     | 0.52              |
| 13:CN:45:LEU:C    | 13:CN:47:LEU:H    | 2.18                     | 0.52              |
| 13:CN:53:ASP:HA   | 13:CN:58:ARG:HH11 | 1.75                     | 0.52              |
| 18:CS:11:ASP:HB2  | 18:CS:14:LEU:HD23 | 1.92                     | 0.52              |
| 19:CT:74:HIS:O    | 19:CT:78:LEU:HG   | 2.10                     | 0.52              |
| 20:CB:161:PHE:HA  | 20:CB:183:PHE:O   | 2.09                     | 0.52              |
| 21:CU:16:ARG:HA   | 21:CU:19:LYS:NZ   | 2.25                     | 0.52              |
| 23:DB:352:A:H3'   | 23:DB:353:C:C6    | 2.45                     | 0.52              |
| 23:DB:1010:A:H4'  | 38:DQ:75:TYR:CD2  | 2.45                     | 0.52              |
| 23:DB:1013:C:H2'  | 23:DB:1014:A:C8   | 2.44                     | 0.52              |
| 23:DB:1441:G:H2'  | 23:DB:1442:U:H6   | 1.73                     | 0.52              |
| 23:DB:1595:C:O2'  | 23:DB:1596:A:H5'  | 2.10                     | 0.52              |
| 23:DB:1599:U:H2'  | 23:DB:1600:C:H6   | 1.75                     | 0.52              |
| 23:DB:1739:A:H2'  | 23:DB:1740:G:H8   | 1.74                     | 0.52              |
| 23:DB:1790:C:O2'  | 25:DC:207:ALA:HB2 | 2.09                     | 0.52              |
| 23:DB:2547:A:H2'  | 23:DB:2548:U:C6   | 2.45                     | 0.52              |
| 23:DB:2599:G:C8   | 25:DC:234:GLY:HA2 | 2.45                     | 0.52              |
| 23:DB:2862:G:H2'  | 23:DB:2863:C:C6   | 2.45                     | 0.52              |
| 36:DO:25:ARG:CB   | 36:DO:94:ARG:HH22 | 2.23                     | 0.52              |
| 36:DO:86:GLY:C    | 36:DO:88:LYS:H    | 2.17                     | 0.52              |
| 41:DT:19:LYS:NZ   | 41:DT:26:LYS:HE2  | 2.25                     | 0.52              |
| 42:DU:13:LEU:HD11 | 42:DU:69:VAL:H    | 1.75                     | 0.52              |
| 44:DX:27:ASN:C    | 44:DX:29:ARG:H    | 2.18                     | 0.52              |
| 45:DY:52:PHE:HB3  | 45:DY:53:MET:CE   | 2.40                     | 0.52              |
| 46:DZ:1:MET:HA    | 46:DZ:9:TYR:CE1   | 2.44                     | 0.52              |
| 49:D2:7:PRO:O     | 49:D2:8:SER:HB3   | 2.09                     | 0.52              |
| 50:D3:29:ARG:O    | 50:D3:30:HIS:C    | 2.53                     | 0.52              |
| 1:AA:625:U:H4'    | 15:AP:16:PHE:CE2  | 2.44                     | 0.52              |
| 1:AA:938:A:H1'    | 1:AA:1376:U:O2'   | 2.10                     | 0.52              |
| 1:AA:1048:G:H4'   | 13:AN:2:LYS:HZ2   | 1.72                     | 0.52              |
| 5:AF:47:LEU:HB3   | 17:AR:65:SER:OG   | 2.10                     | 0.52              |
| 7:AH:84:ILE:N     | 7:AH:84:ILE:HD12  | 2.24                     | 0.52              |
| 8:AI:15:ALA:O     | 8:AI:66:VAL:HG23  | 2.09                     | 0.52              |
| 12:AM:63:VAL:HG12 | 12:AM:68:LEU:HG   | 1.92                     | 0.52              |
| 23:BB:125:A:H4'   | 49:B2:13:ASN:CG   | 2.34                     | 0.52              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:458:G:H1'    | 23:BB:459:U:H5     | 1.73                     | 0.52              |
| 23:BB:781:A:OP1    | 25:BC:216:ARG:NH2  | 2.42                     | 0.52              |
| 23:BB:1745:A:H2'   | 23:BB:1746:A:C8    | 2.45                     | 0.52              |
| 23:BB:1857:G:H2'   | 23:BB:1884:G:N2    | 2.24                     | 0.52              |
| 23:BB:1939:U:H5'   | 23:BB:1939:U:H6    | 1.75                     | 0.52              |
| 23:BB:1986:C:O2'   | 23:BB:1987:A:H5'   | 2.10                     | 0.52              |
| 23:BB:2181:U:H2'   | 23:BB:2182:U:O4'   | 2.10                     | 0.52              |
| 23:BB:2581:G:N2    | 23:BB:2581:G:OP2   | 2.43                     | 0.52              |
| 23:BB:2862:G:H2'   | 23:BB:2863:C:C6    | 2.45                     | 0.52              |
| 25:BC:28:PRO:O     | 25:BC:29:PHE:CB    | 2.58                     | 0.52              |
| 25:BC:52:HIS:O     | 25:BC:53:ILE:HB    | 2.09                     | 0.52              |
| 27:BE:113:VAL:HA   | 27:BE:117:ARG:HD3  | 1.92                     | 0.52              |
| 27:BE:133:LEU:HD12 | 27:BE:136:GLN:OE1  | 2.09                     | 0.52              |
| 28:BF:109:ARG:HG2  | 28:BF:136:ILE:HG13 | 1.92                     | 0.52              |
| 28:BF:133:GLU:OE1  | 28:BF:147:ARG:HD3  | 2.10                     | 0.52              |
| 31:BJ:45:THR:HB    | 38:BQ:63:ARG:HH12  | 1.75                     | 0.52              |
| 33:BL:63:LYS:C     | 50:B3:24:LYS:HZ2   | 2.17                     | 0.52              |
| 33:BL:82:LEU:O     | 33:BL:83:ALA:HB3   | 2.09                     | 0.52              |
| 33:BL:132:ARG:HH11 | 33:BL:132:ARG:HG2  | 1.75                     | 0.52              |
| 36:BO:59:ALA:CB    | 36:BO:63:LYS:HB2   | 2.40                     | 0.52              |
| 38:BQ:87:VAL:HB    | 39:BR:55:ASP:OD2   | 2.10                     | 0.52              |
| 44:BX:22:LEU:HA    | 44:BX:47:ARG:HH12  | 1.75                     | 0.52              |
| 48:B1:22:THR:O     | 48:B1:23:THR:HG23  | 2.10                     | 0.52              |
| 1:CA:246:A:C2      | 1:CA:282:A:C5      | 2.98                     | 0.52              |
| 1:CA:894:G:O2'     | 1:CA:895:G:H5'     | 2.10                     | 0.52              |
| 1:CA:902:G:H2'     | 1:CA:903:G:H8      | 1.74                     | 0.52              |
| 1:CA:1060:U:H5''   | 9:CJ:53:ILE:HG12   | 1.91                     | 0.52              |
| 1:CA:1073:U:O2'    | 1:CA:1074:G:H5'    | 2.10                     | 0.52              |
| 1:CA:1405:G:O2'    | 1:CA:1406:U:H5'    | 2.10                     | 0.52              |
| 2:CC:2:GLN:HE21    | 2:CC:2:GLN:CA      | 2.23                     | 0.52              |
| 4:CE:15:ILE:HG22   | 4:CE:16:ALA:N      | 2.25                     | 0.52              |
| 4:CE:89:THR:CG2    | 4:CE:90:GLY:N      | 2.73                     | 0.52              |
| 6:CG:61:PHE:O      | 6:CG:62:GLU:C      | 2.51                     | 0.52              |
| 8:CI:26:LYS:HG3    | 8:CI:61:ASP:OD2    | 2.10                     | 0.52              |
| 8:CI:56:MET:HG3    | 8:CI:57:VAL:HG23   | 1.92                     | 0.52              |
| 8:CI:114:LYS:HD2   | 8:CI:114:LYS:H     | 1.75                     | 0.52              |
| 11:CL:64:SER:HB2   | 11:CL:81:ILE:HD12  | 1.92                     | 0.52              |
| 15:CP:54:LEU:HD13  | 15:CP:80:LYS:NZ    | 2.25                     | 0.52              |
| 19:CT:43:LYS:HB3   | 19:CT:86:ALA:CB    | 2.39                     | 0.52              |
| 20:CB:57:ASN:HA    | 20:CB:60:ALA:HB3   | 1.90                     | 0.52              |
| 22:DA:44:G:N3      | 22:DA:47:C:N4      | 2.57                     | 0.52              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:109:A:H2'   | 22:DA:110:C:H6     | 1.75                     | 0.52              |
| 23:DB:31:C:O2'    | 23:DB:32:C:H5'     | 2.10                     | 0.52              |
| 23:DB:283:G:H2'   | 23:DB:284:U:H6     | 1.75                     | 0.52              |
| 23:DB:1309:G:H4'  | 49:D2:7:PRO:HB2    | 1.92                     | 0.52              |
| 23:DB:1801:A:H5'  | 23:DB:2203:U:O2'   | 2.09                     | 0.52              |
| 23:DB:2086:U:H2'  | 23:DB:2087:G:H8    | 1.72                     | 0.52              |
| 23:DB:2090:A:O3'  | 46:DZ:49:ARG:HD3   | 2.10                     | 0.52              |
| 23:DB:2370:G:H2'  | 23:DB:2371:G:O4'   | 2.10                     | 0.52              |
| 25:DC:163:ILE:C   | 25:DC:164:VAL:HG22 | 2.34                     | 0.52              |
| 28:DF:32:LYS:HE2  | 28:DF:156:THR:OG1  | 2.09                     | 0.52              |
| 29:DG:151:ARG:HB2 | 29:DG:151:ARG:NH1  | 2.21                     | 0.52              |
| 30:DH:94:ILE:HG23 | 30:DH:98:ASP:CG    | 2.35                     | 0.52              |
| 31:DJ:41:LYS:HE2  | 31:DJ:46:PRO:HD3   | 1.91                     | 0.52              |
| 32:DK:61:VAL:CG1  | 32:DK:87:LEU:HD11  | 2.39                     | 0.52              |
| 32:DK:95:ILE:HG12 | 32:DK:95:ILE:O     | 2.10                     | 0.52              |
| 35:DN:42:LYS:HE3  | 35:DN:42:LYS:CA    | 2.39                     | 0.52              |
| 35:DN:86:ARG:HH11 | 35:DN:86:ARG:CB    | 2.20                     | 0.52              |
| 37:DP:27:VAL:HG23 | 37:DP:86:LYS:CB    | 2.40                     | 0.52              |
| 43:DW:60:ALA:HB3  | 43:DW:80:SER:CA    | 2.39                     | 0.52              |
| 43:DW:67:LYS:CD   | 43:DW:71:LYS:H     | 2.23                     | 0.52              |
| 45:DY:1:ALA:HB1   | 45:DY:37:ARG:HB3   | 1.92                     | 0.52              |
| 1:AA:140:U:H2'    | 1:AA:141:G:H8      | 1.73                     | 0.51              |
| 1:AA:648:A:H2'    | 1:AA:649:A:C8      | 2.45                     | 0.51              |
| 1:AA:978:A:HO2'   | 1:AA:1322:C:H5     | 1.55                     | 0.51              |
| 1:AA:1060:U:H4'   | 9:AJ:54:SER:HB2    | 1.92                     | 0.51              |
| 4:AE:104:ILE:CD1  | 4:AE:114:LEU:HB2   | 2.40                     | 0.51              |
| 23:BB:189:G:H2'   | 23:BB:205:G:N2     | 2.26                     | 0.51              |
| 23:BB:208:C:H2'   | 23:BB:209:C:C6     | 2.45                     | 0.51              |
| 23:BB:233:A:H61   | 23:BB:428:A:H61    | 1.57                     | 0.51              |
| 23:BB:995:C:OP2   | 38:BQ:53:LYS:HE2   | 2.08                     | 0.51              |
| 23:BB:1228:G:H2'  | 23:BB:1229:C:C6    | 2.45                     | 0.51              |
| 23:BB:1430:G:H2'  | 23:BB:1431:A:H8    | 1.74                     | 0.51              |
| 23:BB:1916:A:H2'  | 23:BB:1917:U:C6    | 2.44                     | 0.51              |
| 23:BB:2052:A:C5'  | 26:BD:148:GLN:H    | 2.21                     | 0.51              |
| 23:BB:2195:U:H2'  | 23:BB:2196:C:H6    | 1.76                     | 0.51              |
| 25:BC:248:GLY:C   | 25:BC:250:GLN:H    | 2.18                     | 0.51              |
| 27:BE:47:LYS:HD3  | 27:BE:47:LYS:N     | 2.12                     | 0.51              |
| 27:BE:132:LYS:HD3 | 27:BE:133:LEU:HD22 | 1.91                     | 0.51              |
| 27:BE:152:GLU:H   | 27:BE:171:ASP:HB3  | 1.75                     | 0.51              |
| 28:BF:77:LYS:NZ   | 28:BF:79:ARG:HE    | 2.08                     | 0.51              |
| 30:BH:125:THR:OG1 | 30:BH:146:VAL:HB   | 2.10                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BJ:81:ILE:HG23  | 31:BJ:82:GLY:N     | 2.25                     | 0.51              |
| 31:BJ:122:LEU:HD12 | 31:BJ:123:LYS:N    | 2.24                     | 0.51              |
| 32:BK:47:ILE:HG23  | 32:BK:48:PRO:CD    | 2.40                     | 0.51              |
| 34:BM:3:GLN:C      | 34:BM:5:LYS:N      | 2.66                     | 0.51              |
| 38:BQ:47:ARG:HH21  | 38:BQ:51:GLN:N     | 2.08                     | 0.51              |
| 40:BS:2:GLU:OE1    | 40:BS:108:SER:HB3  | 2.10                     | 0.51              |
| 43:BW:45:HIS:ND1   | 43:BW:64:GLY:HA3   | 2.24                     | 0.51              |
| 46:BZ:5:ILE:HD12   | 46:BZ:5:ILE:N      | 2.17                     | 0.51              |
| 50:B3:23:HIS:CD2   | 50:B3:47:ALA:HA    | 2.45                     | 0.51              |
| 51:B4:15:LYS:HB2   | 51:B4:26:ILE:HD11  | 1.91                     | 0.51              |
| 1:CA:252:U:H2'     | 1:CA:253:A:H8      | 1.74                     | 0.51              |
| 1:CA:280:C:H1'     | 16:CQ:39:ARG:NH1   | 2.25                     | 0.51              |
| 1:CA:940:C:H2'     | 1:CA:941:G:C8      | 2.45                     | 0.51              |
| 1:CA:960:U:O2'     | 1:CA:961:U:P       | 2.68                     | 0.51              |
| 1:CA:1023:U:H2'    | 1:CA:1024:G:H8     | 1.75                     | 0.51              |
| 3:CD:2:ARG:O       | 3:CD:3:TYR:HB3     | 2.10                     | 0.51              |
| 3:CD:121:ALA:HA    | 3:CD:145:ARG:HG3   | 1.93                     | 0.51              |
| 6:CG:4:ARG:HB2     | 6:CG:4:ARG:NH1     | 2.25                     | 0.51              |
| 6:CG:63:VAL:CG1    | 6:CG:126:ALA:HB1   | 2.40                     | 0.51              |
| 7:CH:45:ILE:HD13   | 7:CH:60:LEU:HD11   | 1.91                     | 0.51              |
| 10:CK:70:ALA:HA    | 10:CK:73:VAL:HG22  | 1.91                     | 0.51              |
| 13:CN:50:LEU:CD1   | 13:CN:51:PRO:HD3   | 2.40                     | 0.51              |
| 13:CN:65:GLN:HG2   | 13:CN:82:LYS:HG3   | 1.92                     | 0.51              |
| 20:CB:31:PHE:N     | 20:CB:41:ASN:HB2   | 2.25                     | 0.51              |
| 23:DB:86:G:OP1     | 42:DU:28:LEU:HD22  | 2.10                     | 0.51              |
| 23:DB:192:C:C2'    | 23:DB:193:U:H5'    | 2.39                     | 0.51              |
| 23:DB:656:G:H2'    | 23:DB:657:U:C6     | 2.45                     | 0.51              |
| 23:DB:771:G:O2'    | 23:DB:772:C:H5'    | 2.10                     | 0.51              |
| 23:DB:845:A:N1     | 23:DB:847:U:H1'    | 2.25                     | 0.51              |
| 23:DB:1021:A:H61   | 23:DB:1142:A:H61   | 1.52                     | 0.51              |
| 23:DB:1563:U:H2'   | 23:DB:1564:C:C6    | 2.45                     | 0.51              |
| 23:DB:1639:C:H2'   | 23:DB:1640:A:C5'   | 2.33                     | 0.51              |
| 23:DB:1654:A:O2'   | 26:DD:118:PHE:O    | 2.27                     | 0.51              |
| 23:DB:2440:C:H5'   | 55:DB:3424:HOH:O   | 2.10                     | 0.51              |
| 23:DB:2599:G:N7    | 25:DC:234:GLY:HA2  | 2.26                     | 0.51              |
| 23:DB:2755:C:H2'   | 51:D4:19:ARG:NH2   | 2.25                     | 0.51              |
| 25:DC:226:PRO:HG3  | 25:DC:232:GLY:C    | 2.35                     | 0.51              |
| 26:DD:146:ILE:CG1  | 26:DD:155:VAL:HG13 | 2.40                     | 0.51              |
| 27:DE:142:ALA:C    | 27:DE:143:LEU:HD13 | 2.34                     | 0.51              |
| 31:DJ:61:LYS:HA    | 31:DJ:61:LYS:HE3   | 1.92                     | 0.51              |
| 32:DK:105:ARG:O    | 32:DK:108:ARG:HB3  | 2.10                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:DL:109:LYS:HG2  | 33:DL:126:ARG:HH11 | 1.74                     | 0.51              |
| 35:DN:107:ASN:HD21 | 40:DS:40:ASN:HB3   | 1.75                     | 0.51              |
| 38:DQ:38:VAL:HA    | 38:DQ:41:ALA:HB3   | 1.92                     | 0.51              |
| 39:DR:97:LYS:O     | 39:DR:98:ILE:HB    | 2.10                     | 0.51              |
| 40:DS:46:LEU:O     | 40:DS:50:VAL:HG22  | 2.10                     | 0.51              |
| 42:DU:15:GLY:C     | 42:DU:17:ASP:H     | 2.18                     | 0.51              |
| 1:AA:35:G:H2'      | 1:AA:36:C:C6       | 2.46                     | 0.51              |
| 1:AA:250:A:H1'     | 1:AA:252:U:C5      | 2.45                     | 0.51              |
| 1:AA:590:U:OP1     | 7:AH:30:LYS:HG2    | 2.10                     | 0.51              |
| 1:AA:783:C:O2'     | 1:AA:784:A:H5'     | 2.10                     | 0.51              |
| 1:AA:1284:C:H3'    | 1:AA:1285:A:C5'    | 2.35                     | 0.51              |
| 3:AD:145:ARG:HB3   | 3:AD:147:LYS:HE3   | 1.92                     | 0.51              |
| 8:AI:122:ARG:HG3   | 8:AI:122:ARG:NH1   | 2.21                     | 0.51              |
| 11:AL:80:LEU:O     | 11:AL:97:VAL:HG23  | 2.09                     | 0.51              |
| 11:AL:119:LYS:HG3  | 11:AL:119:LYS:O    | 2.11                     | 0.51              |
| 13:AN:30:ILE:HD12  | 13:AN:30:ILE:N     | 2.19                     | 0.51              |
| 16:AQ:75:VAL:HG23  | 16:AQ:76:ARG:N     | 2.25                     | 0.51              |
| 17:AR:31:TYR:CG    | 17:AR:54:LEU:HD21  | 2.45                     | 0.51              |
| 23:BB:167:A:H2'    | 23:BB:168:G:O4'    | 2.10                     | 0.51              |
| 23:BB:1081:U:H5''  | 52:BI:126:ARG:HD2  | 1.92                     | 0.51              |
| 23:BB:1438:U:H5'   | 23:BB:1516:G:O2'   | 2.10                     | 0.51              |
| 23:BB:1563:U:H2'   | 23:BB:1564:C:C6    | 2.45                     | 0.51              |
| 25:BC:180:MET:HB2  | 25:BC:265:PHE:HB2  | 1.93                     | 0.51              |
| 25:BC:250:GLN:O    | 25:BC:251:THR:HB   | 2.09                     | 0.51              |
| 26:BD:18:ASP:OD2   | 26:BD:20:VAL:HG13  | 2.09                     | 0.51              |
| 27:BE:173:THR:HA   | 27:BE:201:ALA:O    | 2.11                     | 0.51              |
| 29:BG:126:THR:C    | 29:BG:128:THR:H    | 2.17                     | 0.51              |
| 30:BH:37:VAL:H     | 30:BH:38:PRO:CD    | 2.11                     | 0.51              |
| 30:BH:89:LYS:HZ3   | 30:BH:90:LEU:H     | 1.58                     | 0.51              |
| 37:BP:26:GLU:CA    | 37:BP:46:VAL:HG13  | 2.38                     | 0.51              |
| 37:BP:28:LYS:O     | 37:BP:30:TRP:N     | 2.43                     | 0.51              |
| 37:BP:52:ARG:CB    | 37:BP:60:VAL:HG11  | 2.25                     | 0.51              |
| 38:BQ:75:TYR:CZ    | 38:BQ:79:ILE:HD11  | 2.44                     | 0.51              |
| 38:BQ:92:LYS:HD3   | 38:BQ:92:LYS:C     | 2.35                     | 0.51              |
| 40:BS:89:ALA:O     | 40:BS:90:LYS:HB2   | 2.10                     | 0.51              |
| 41:BT:25:GLU:HG3   | 41:BT:26:LYS:N     | 2.25                     | 0.51              |
| 41:BT:34:VAL:CG1   | 41:BT:43:ILE:HD11  | 2.39                     | 0.51              |
| 42:BU:5:ARG:CG     | 42:BU:6:ARG:N      | 2.73                     | 0.51              |
| 52:BI:112:LYS:O    | 52:BI:116:MET:HG3  | 2.09                     | 0.51              |
| 1:CA:1165:U:H2'    | 1:CA:1166:G:O4'    | 2.10                     | 0.51              |
| 7:CH:104:SER:O     | 7:CH:122:GLY:HA3   | 2.10                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:CI:22:PRO:HA    | 8:CI:60:LEU:HB3   | 1.92                     | 0.51              |
| 15:CP:23:ASP:OD1  | 15:CP:25:ARG:HB2  | 2.10                     | 0.51              |
| 17:CR:33:THR:HG21 | 17:CR:37:LYS:HG2  | 1.92                     | 0.51              |
| 23:DB:753:A:H2'   | 23:DB:754:U:C6    | 2.45                     | 0.51              |
| 23:DB:1107:G:O2'  | 23:DB:1108:U:H5'  | 2.10                     | 0.51              |
| 23:DB:1161:C:H2'  | 23:DB:1162:G:H8   | 1.76                     | 0.51              |
| 23:DB:1560:G:H2'  | 23:DB:1561:C:C6   | 2.45                     | 0.51              |
| 23:DB:2066:C:O2'  | 23:DB:2067:G:H5'  | 2.11                     | 0.51              |
| 23:DB:2336:A:C1'  | 23:DB:2337:G:OP1  | 2.56                     | 0.51              |
| 23:DB:2877:G:O2'  | 23:DB:2878:U:H5'  | 2.10                     | 0.51              |
| 26:DD:56:LYS:HZ2  | 26:DD:59:ARG:HB2  | 1.75                     | 0.51              |
| 31:DJ:120:ARG:C   | 31:DJ:121:LYS:HE3 | 2.35                     | 0.51              |
| 32:DK:110:GLU:HA  | 32:DK:113:MET:HE3 | 1.91                     | 0.51              |
| 35:DN:14:SER:HA   | 35:DN:17:ARG:HH22 | 1.75                     | 0.51              |
| 37:DP:100:ARG:HD2 | 37:DP:100:ARG:H   | 1.76                     | 0.51              |
| 39:DR:76:LYS:HD2  | 39:DR:90:ARG:HB3  | 1.90                     | 0.51              |
| 47:D0:29:VAL:CG2  | 47:D0:32:THR:H    | 2.24                     | 0.51              |
| 1:AA:531:U:H5'    | 1:AA:531:U:H6     | 1.75                     | 0.51              |
| 1:AA:1108:G:H5'   | 2:AC:175:HIS:CD2  | 2.46                     | 0.51              |
| 1:AA:1464:U:H2'   | 1:AA:1465:A:C8    | 2.45                     | 0.51              |
| 1:AA:1475:G:OP1   | 23:BB:1689:A:H1'  | 2.10                     | 0.51              |
| 1:AA:1512:U:O2'   | 1:AA:1513:A:H5'   | 2.10                     | 0.51              |
| 2:AC:75:VAL:HG12  | 2:AC:75:VAL:O     | 2.10                     | 0.51              |
| 10:AK:111:ASP:O   | 17:AR:72:ARG:HD3  | 2.10                     | 0.51              |
| 11:AL:22:ALA:HB2  | 11:AL:56:LEU:CD2  | 2.39                     | 0.51              |
| 23:BB:163:C:H5'   | 23:BB:163:C:O2    | 2.10                     | 0.51              |
| 23:BB:587:C:N3    | 33:BL:38:GLN:CB   | 2.73                     | 0.51              |
| 23:BB:869:G:H2'   | 23:BB:870:U:C6    | 2.45                     | 0.51              |
| 23:BB:1205:A:C4'  | 23:BB:1206:G:OP2  | 2.59                     | 0.51              |
| 23:BB:1516:G:O2'  | 23:BB:1517:G:H5'  | 2.10                     | 0.51              |
| 23:BB:1595:C:O2'  | 23:BB:1596:A:H5'  | 2.10                     | 0.51              |
| 23:BB:1812:U:H2'  | 23:BB:1813:G:H8   | 1.75                     | 0.51              |
| 23:BB:2285:C:H41  | 48:B1:24:LYS:HZ2  | 1.58                     | 0.51              |
| 23:BB:2518:A:N3   | 23:BB:2518:A:H2'  | 2.25                     | 0.51              |
| 23:BB:2869:G:H2'  | 23:BB:2870:C:H6   | 1.75                     | 0.51              |
| 24:BV:23:ALA:O    | 24:BV:24:ASN:HB2  | 2.11                     | 0.51              |
| 25:BC:81:GLU:HB3  | 25:BC:90:ILE:HG22 | 1.93                     | 0.51              |
| 26:BD:46:ARG:HA   | 26:BD:81:GLU:O    | 2.09                     | 0.51              |
| 28:BF:37:MET:HE3  | 28:BF:56:LEU:CD1  | 2.36                     | 0.51              |
| 29:BG:53:PRO:HG2  | 29:BG:61:TRP:HA   | 1.92                     | 0.51              |
| 33:BL:21:ARG:HB3  | 33:BL:21:ARG:HH11 | 1.74                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 37:BP:64:SER:HA    | 37:BP:72:VAL:HG12 | 1.91                     | 0.51              |
| 38:BQ:30:VAL:O     | 38:BQ:33:VAL:HG12 | 2.11                     | 0.51              |
| 39:BR:51:VAL:HG12  | 39:BR:53:PHE:H    | 1.74                     | 0.51              |
| 51:B4:13:ASN:N     | 51:B4:13:ASN:HD22 | 2.08                     | 0.51              |
| 52:BI:27:LEU:HD23  | 52:BI:27:LEU:N    | 2.18                     | 0.51              |
| 1:CA:73:C:H2'      | 1:CA:74:A:C8      | 2.45                     | 0.51              |
| 1:CA:217:C:O2'     | 1:CA:218:U:H5'    | 2.10                     | 0.51              |
| 1:CA:392:C:H2'     | 1:CA:393:A:H8     | 1.75                     | 0.51              |
| 1:CA:442:G:H2'     | 1:CA:443:C:C6     | 2.45                     | 0.51              |
| 1:CA:648:A:H2'     | 1:CA:649:A:C8     | 2.46                     | 0.51              |
| 1:CA:837:U:H2'     | 1:CA:838:G:H8     | 1.75                     | 0.51              |
| 1:CA:864:A:H2'     | 1:CA:865:A:C8     | 2.46                     | 0.51              |
| 1:CA:1151:A:HO2'   | 1:CA:1152:A:H5''  | 1.74                     | 0.51              |
| 1:CA:1275:A:H2'    | 1:CA:1276:G:O4'   | 2.11                     | 0.51              |
| 1:CA:1477:U:H2'    | 1:CA:1478:U:C6    | 2.46                     | 0.51              |
| 2:CC:33:ASP:OD1    | 2:CC:37:LYS:HE2   | 2.10                     | 0.51              |
| 7:CH:38:VAL:HG13   | 7:CH:39:LEU:HD22  | 1.93                     | 0.51              |
| 10:CK:109:ILE:HD12 | 10:CK:109:ILE:N   | 2.25                     | 0.51              |
| 11:CL:56:LEU:HD12  | 11:CL:60:PHE:HB2  | 1.92                     | 0.51              |
| 23:DB:146:A:H2'    | 23:DB:147:C:C6    | 2.44                     | 0.51              |
| 23:DB:1050:A:O2'   | 23:DB:2752:C:H1'  | 2.10                     | 0.51              |
| 23:DB:1534:U:O2'   | 23:DB:1535:A:H8   | 1.93                     | 0.51              |
| 23:DB:1745:A:H2'   | 23:DB:1746:A:C8   | 2.45                     | 0.51              |
| 23:DB:1812:U:H2'   | 23:DB:1813:G:H8   | 1.75                     | 0.51              |
| 23:DB:2018:G:H1'   | 38:DQ:32:ARG:NH2  | 2.24                     | 0.51              |
| 23:DB:2033:A:H1'   | 23:DB:2035:G:OP2  | 2.11                     | 0.51              |
| 23:DB:2065:C:H2'   | 23:DB:2066:C:H6   | 1.74                     | 0.51              |
| 23:DB:2281:A:O2'   | 23:DB:2282:G:H5'  | 2.11                     | 0.51              |
| 23:DB:2327:A:H2'   | 23:DB:2328:A:C8   | 2.46                     | 0.51              |
| 23:DB:2394:C:H5''  | 33:DL:64:PHE:CE2  | 2.46                     | 0.51              |
| 23:DB:2484:G:H21   | 34:DM:118:LYS:HG2 | 1.75                     | 0.51              |
| 24:DV:30:ILE:HG12  | 24:DV:91:PHE:CB   | 2.38                     | 0.51              |
| 28:DF:66:ILE:HG22  | 28:DF:66:ILE:O    | 2.11                     | 0.51              |
| 29:DG:10:VAL:HG23  | 29:DG:47:ASN:O    | 2.10                     | 0.51              |
| 30:DH:4:ILE:HD13   | 30:DH:4:ILE:N     | 2.25                     | 0.51              |
| 31:DJ:136:GLN:N    | 31:DJ:137:PRO:CD  | 2.73                     | 0.51              |
| 33:DL:109:LYS:HE2  | 33:DL:126:ARG:NH1 | 2.26                     | 0.51              |
| 34:DM:61:GLY:HA3   | 34:DM:105:MET:HB2 | 1.91                     | 0.51              |
| 34:DM:97:GLN:N     | 34:DM:98:PRO:HD3  | 2.25                     | 0.51              |
| 36:DO:18:LEU:HD21  | 36:DO:43:ASN:HD22 | 1.74                     | 0.51              |
| 37:DP:54:LEU:HD12  | 37:DP:54:LEU:N    | 2.25                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:DP:90:ALA:HB3   | 37:DP:111:GLU:HB2  | 1.91                     | 0.51              |
| 40:DS:9:HIS:O      | 40:DS:10:ALA:HB3   | 2.09                     | 0.51              |
| 43:DW:10:ARG:NH1   | 43:DW:10:ARG:HA    | 2.26                     | 0.51              |
| 45:DY:10:ARG:HG2   | 45:DY:31:ILE:HG21  | 1.92                     | 0.51              |
| 47:D0:36:LYS:HB2   | 47:D0:41:HIS:ND1   | 2.25                     | 0.51              |
| 47:D0:42:ILE:O     | 47:D0:42:ILE:HG23  | 2.11                     | 0.51              |
| 52:DI:53:PRO:CG    | 52:DI:77:VAL:HG11  | 2.39                     | 0.51              |
| 1:AA:676:A:O2'     | 1:AA:677:U:H5'     | 2.10                     | 0.51              |
| 1:AA:883:C:O2'     | 1:AA:884:U:H5'     | 2.09                     | 0.51              |
| 1:AA:1348:U:H4'    | 8:AI:121:ARG:HH11  | 1.76                     | 0.51              |
| 3:AD:84:ASN:HD22   | 3:AD:87:GLU:N      | 2.01                     | 0.51              |
| 4:AE:14:LEU:HA     | 4:AE:36:THR:HG22   | 1.91                     | 0.51              |
| 6:AG:72:VAL:HB     | 6:AG:144:ALA:CB    | 2.41                     | 0.51              |
| 11:AL:3:VAL:HG23   | 11:AL:4:ASN:OD1    | 2.10                     | 0.51              |
| 20:AB:116:LEU:HD12 | 20:AB:143:LEU:HD12 | 1.93                     | 0.51              |
| 20:AB:216:VAL:O    | 20:AB:220:VAL:HG23 | 2.11                     | 0.51              |
| 21:AU:5:VAL:HG12   | 21:AU:6:ARG:N      | 2.25                     | 0.51              |
| 23:BB:165:A:H2'    | 23:BB:166:U:O4'    | 2.11                     | 0.51              |
| 23:BB:642:U:H2'    | 23:BB:644:A:OP2    | 2.10                     | 0.51              |
| 23:BB:740:C:H5''   | 23:BB:1784:A:OP1   | 2.11                     | 0.51              |
| 23:BB:786:C:O2'    | 23:BB:787:C:H5'    | 2.10                     | 0.51              |
| 23:BB:1330:C:H2'   | 23:BB:1331:G:H8    | 1.76                     | 0.51              |
| 23:BB:1560:G:H2'   | 23:BB:1561:C:C6    | 2.45                     | 0.51              |
| 23:BB:2742:G:O2'   | 23:BB:2743:U:H5'   | 2.11                     | 0.51              |
| 23:BB:2771:C:H2'   | 23:BB:2772:C:H6    | 1.76                     | 0.51              |
| 23:BB:2784:U:H4'   | 26:BD:41:ALA:O     | 2.10                     | 0.51              |
| 26:BD:55:LYS:HB2   | 26:BD:55:LYS:NZ    | 2.25                     | 0.51              |
| 26:BD:67:HIS:O     | 26:BD:71:ALA:HB3   | 2.10                     | 0.51              |
| 29:BG:51:PHE:HB3   | 29:BG:64:ALA:HB1   | 1.91                     | 0.51              |
| 33:BL:111:ILE:H    | 33:BL:111:ILE:CD1  | 2.23                     | 0.51              |
| 37:BP:23:ASP:O     | 37:BP:25:VAL:HG23  | 2.09                     | 0.51              |
| 37:BP:29:VAL:O     | 37:BP:30:TRP:C     | 2.53                     | 0.51              |
| 39:BR:18:GLN:HA    | 39:BR:99:THR:HA    | 1.92                     | 0.51              |
| 43:BW:3:LYS:HD2    | 43:BW:3:LYS:N      | 2.26                     | 0.51              |
| 46:BZ:3:LYS:HB2    | 46:BZ:51:VAL:CG2   | 2.29                     | 0.51              |
| 1:CA:81:A:H2'      | 1:CA:82:G:C8       | 2.45                     | 0.51              |
| 1:CA:146:G:O2'     | 1:CA:147:G:H5'     | 2.11                     | 0.51              |
| 1:CA:250:A:H1'     | 1:CA:252:U:C5      | 2.45                     | 0.51              |
| 1:CA:251:G:H4'     | 1:CA:252:U:H5'     | 1.92                     | 0.51              |
| 1:CA:333:U:H2'     | 1:CA:334:C:H6      | 1.74                     | 0.51              |
| 1:CA:376:G:C5'     | 15:CP:5:ARG:HD3    | 2.40                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:987:G:H2'     | 1:CA:988:G:C8      | 2.45                     | 0.51              |
| 1:CA:1006:G:H2'    | 1:CA:1007:U:C6     | 2.45                     | 0.51              |
| 1:CA:1464:U:H2'    | 1:CA:1465:A:C8     | 2.45                     | 0.51              |
| 3:CD:101:VAL:O     | 3:CD:104:MET:HB2   | 2.11                     | 0.51              |
| 3:CD:202:LEU:C     | 3:CD:204:SER:H     | 2.17                     | 0.51              |
| 4:CE:80:LEU:CD2    | 4:CE:122:VAL:HG11  | 2.40                     | 0.51              |
| 9:CJ:5:ARG:HG2     | 9:CJ:5:ARG:O       | 2.09                     | 0.51              |
| 12:CM:79:LEU:CD2   | 12:CM:86:ARG:HE    | 2.23                     | 0.51              |
| 14:CO:31:LEU:O     | 14:CO:35:ILE:HG12  | 2.10                     | 0.51              |
| 15:CP:12:LYS:O     | 15:CP:13:LYS:HB2   | 2.10                     | 0.51              |
| 19:CT:49:ALA:O     | 19:CT:52:GLU:HB3   | 2.10                     | 0.51              |
| 23:DB:396:G:H2'    | 23:DB:397:U:H6     | 1.75                     | 0.51              |
| 23:DB:441:U:H2'    | 23:DB:442:G:C8     | 2.45                     | 0.51              |
| 23:DB:919:U:O5'    | 23:DB:919:U:H6     | 1.94                     | 0.51              |
| 23:DB:1150:C:O2'   | 23:DB:1151:A:H5'   | 2.11                     | 0.51              |
| 23:DB:1360:G:H2'   | 23:DB:1361:G:C5'   | 2.41                     | 0.51              |
| 23:DB:2053:G:O2'   | 23:DB:2054:A:H5'   | 2.11                     | 0.51              |
| 23:DB:2688:G:H1'   | 23:DB:2721:A:N6    | 2.25                     | 0.51              |
| 24:DV:2:PHE:HB3    | 24:DV:50:MET:SD    | 2.50                     | 0.51              |
| 27:DE:4:VAL:HA     | 27:DE:14:VAL:HG22  | 1.92                     | 0.51              |
| 27:DE:77:ILE:HG23  | 27:DE:78:TRP:CD1   | 2.45                     | 0.51              |
| 28:DF:135:ILE:HG23 | 28:DF:136:ILE:H    | 1.75                     | 0.51              |
| 31:DJ:77:HIS:HB2   | 31:DJ:85:LYS:CE    | 2.39                     | 0.51              |
| 31:DJ:106:LYS:C    | 31:DJ:108:MET:H    | 2.18                     | 0.51              |
| 35:DN:61:ALA:O     | 35:DN:64:ARG:HB3   | 2.09                     | 0.51              |
| 1:AA:394:G:H2'     | 1:AA:395:C:H6      | 1.75                     | 0.51              |
| 1:AA:499:A:C2      | 1:AA:546:A:N3      | 2.79                     | 0.51              |
| 1:AA:1460:C:H2'    | 1:AA:1461:G:O4'    | 2.11                     | 0.51              |
| 2:AC:150:VAL:HG12  | 2:AC:151:GLU:N     | 2.25                     | 0.51              |
| 3:AD:112:GLU:OE2   | 3:AD:153:ARG:HD3   | 2.11                     | 0.51              |
| 8:AI:34:LEU:HD11   | 8:AI:47:VAL:CG2    | 2.40                     | 0.51              |
| 15:AP:20:VAL:HG21  | 15:AP:32:PHE:CD2   | 2.45                     | 0.51              |
| 20:AB:132:GLU:O    | 20:AB:136:ARG:HG3  | 2.10                     | 0.51              |
| 22:BA:114:C:H4'    | 36:BO:49:VAL:HG11  | 1.91                     | 0.51              |
| 23:BB:161:A:H3'    | 23:BB:162:U:C5'    | 2.25                     | 0.51              |
| 23:BB:2033:A:H1'   | 23:BB:2035:G:OP2   | 2.11                     | 0.51              |
| 23:BB:2073:C:H5''  | 25:BC:227:VAL:HG23 | 1.92                     | 0.51              |
| 23:BB:2093:G:N7    | 23:BB:2225:A:H2'   | 2.26                     | 0.51              |
| 23:BB:2322:A:N6    | 23:BB:2333:A:H62   | 2.09                     | 0.51              |
| 23:BB:2469:A:H5''  | 34:BM:55:ARG:HD2   | 1.93                     | 0.51              |
| 23:BB:2547:A:H2'   | 23:BB:2548:U:C6    | 2.44                     | 0.51              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:2718:G:O2'   | 23:BB:2719:G:H5'   | 2.09                     | 0.51              |
| 25:BC:153:LEU:HD13 | 25:BC:161:VAL:HG23 | 1.93                     | 0.51              |
| 26:BD:167:ASN:N    | 26:BD:167:ASN:ND2  | 2.58                     | 0.51              |
| 29:BG:137:LYS:HA   | 29:BG:140:ILE:CG1  | 2.40                     | 0.51              |
| 31:BJ:56:VAL:HG12  | 31:BJ:57:LEU:N     | 2.25                     | 0.51              |
| 31:BJ:58:ASN:O     | 31:BJ:126:ALA:HA   | 2.10                     | 0.51              |
| 33:BL:61:LEU:O     | 50:B3:11:LYS:NZ    | 2.43                     | 0.51              |
| 33:BL:82:LEU:HD21  | 33:BL:92:LEU:HD12  | 1.92                     | 0.51              |
| 34:BM:8:LYS:HB2    | 34:BM:12:MET:CE    | 2.41                     | 0.51              |
| 38:BQ:99:VAL:HG23  | 38:BQ:100:PHE:CD1  | 2.44                     | 0.51              |
| 39:BR:90:ARG:HH12  | 39:BR:91:GLN:C     | 2.18                     | 0.51              |
| 46:BZ:69:SER:HB3   | 46:BZ:70:LYS:HE3   | 1.92                     | 0.51              |
| 48:B1:34:GLU:O     | 48:B1:35:LEU:HB3   | 2.10                     | 0.51              |
| 1:CA:541:G:H2'     | 1:CA:542:G:H8      | 1.75                     | 0.51              |
| 1:CA:602:A:O2'     | 1:CA:603:U:H5'     | 2.10                     | 0.51              |
| 1:CA:629:A:H2'     | 1:CA:630:A:O4'     | 2.11                     | 0.51              |
| 11:CL:23:LEU:CD2   | 11:CL:58:ASN:HD22  | 2.18                     | 0.51              |
| 13:CN:15:LEU:O     | 13:CN:19:TYR:HB2   | 2.10                     | 0.51              |
| 13:CN:51:PRO:CB    | 13:CN:54:SER:HB3   | 2.40                     | 0.51              |
| 19:CT:38:ILE:HD13  | 19:CT:85:LEU:HD23  | 1.93                     | 0.51              |
| 20:CB:69:VAL:HB    | 20:CB:162:VAL:HB   | 1.91                     | 0.51              |
| 21:CU:14:ALA:HB3   | 21:CU:16:ARG:HH12  | 1.74                     | 0.51              |
| 22:DA:25:U:OP1     | 22:DA:25:U:H3'     | 2.10                     | 0.51              |
| 22:DA:29:A:OP1     | 22:DA:29:A:C8      | 2.64                     | 0.51              |
| 22:DA:114:C:O2'    | 36:DO:49:VAL:HG23  | 2.10                     | 0.51              |
| 23:DB:61:C:OP2     | 44:DX:44:LYS:HB2   | 2.11                     | 0.51              |
| 23:DB:394:C:O2'    | 23:DB:395:U:H5'    | 2.11                     | 0.51              |
| 23:DB:720:U:H2'    | 23:DB:721:A:C8     | 2.46                     | 0.51              |
| 23:DB:1029:A:H3'   | 23:DB:1030:C:H6    | 1.76                     | 0.51              |
| 23:DB:1315:C:H2'   | 23:DB:1316:U:C6    | 2.46                     | 0.51              |
| 23:DB:1656:C:H2'   | 23:DB:1657:U:H6    | 1.74                     | 0.51              |
| 23:DB:2328:A:H2'   | 23:DB:2329:U:H6    | 1.71                     | 0.51              |
| 23:DB:2700:A:H2'   | 23:DB:2701:U:H6    | 1.76                     | 0.51              |
| 25:DC:243:PRO:O    | 25:DC:244:VAL:HG23 | 2.11                     | 0.51              |
| 27:DE:47:LYS:O     | 27:DE:49:ARG:HG2   | 2.10                     | 0.51              |
| 27:DE:139:LYS:HA   | 27:DE:143:LEU:CD2  | 2.40                     | 0.51              |
| 31:DJ:14:ASP:H     | 31:DJ:53:TYR:HD1   | 1.57                     | 0.51              |
| 31:DJ:53:TYR:HA    | 31:DJ:121:LYS:HB3  | 1.93                     | 0.51              |
| 40:DS:3:THR:OG1    | 40:DS:107:VAL:HG23 | 2.10                     | 0.51              |
| 41:DT:17:SER:H     | 41:DT:20:ALA:CB    | 2.22                     | 0.51              |
| 41:DT:55:VAL:CG2   | 41:DT:56:GLU:H     | 2.15                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:DU:78:LYS:HD2   | 42:DU:96:LYS:CG    | 2.41                     | 0.51              |
| 43:DW:44:PHE:HD2   | 43:DW:77:LYS:HB3   | 1.75                     | 0.51              |
| 52:DI:72:THR:CG2   | 52:DI:112:LYS:HD2  | 2.40                     | 0.51              |
| 52:DI:105:LEU:CD1  | 52:DI:129:GLU:HG2  | 2.37                     | 0.51              |
| 1:AA:212:G:H2'     | 1:AA:213:G:C8      | 2.46                     | 0.51              |
| 1:AA:537:G:H2'     | 1:AA:538:G:C8      | 2.45                     | 0.51              |
| 1:AA:1448:C:H2'    | 1:AA:1449:C:H6     | 1.74                     | 0.51              |
| 2:AC:41:TYR:HA     | 2:AC:44:LYS:HD3    | 1.92                     | 0.51              |
| 3:AD:104:MET:SD    | 3:AD:179:GLY:HA3   | 2.51                     | 0.51              |
| 4:AE:84:VAL:HG21   | 4:AE:142:GLY:O     | 2.11                     | 0.51              |
| 6:AG:117:LEU:HD13  | 6:AG:117:LEU:O     | 2.11                     | 0.51              |
| 7:AH:79:ARG:HB2    | 7:AH:80:PRO:HD2    | 1.92                     | 0.51              |
| 18:AS:3:SER:O      | 18:AS:4:LEU:HG     | 2.11                     | 0.51              |
| 20:AB:102:ASN:OD1  | 20:AB:105:THR:HG22 | 2.10                     | 0.51              |
| 23:BB:589:U:H1'    | 27:BE:88:ARG:NH2   | 2.26                     | 0.51              |
| 23:BB:811:U:O5'    | 33:BL:31:GLY:HA2   | 2.11                     | 0.51              |
| 23:BB:999:U:O2'    | 23:BB:1000:A:H5'   | 2.11                     | 0.51              |
| 23:BB:1230:A:H2'   | 23:BB:1231:U:C6    | 2.46                     | 0.51              |
| 23:BB:1599:U:H2'   | 23:BB:1600:C:H6    | 1.75                     | 0.51              |
| 23:BB:2262:U:H4'   | 23:BB:2328:A:C2    | 2.46                     | 0.51              |
| 55:BB:3366:HOH:O   | 35:BN:15:SER:HB3   | 2.11                     | 0.51              |
| 25:BC:155:ARG:O    | 25:BC:156:SER:C    | 2.54                     | 0.51              |
| 28:BF:150:GLY:O    | 28:BF:151:LEU:HD12 | 2.11                     | 0.51              |
| 30:BH:8:LYS:HB3    | 30:BH:14:SER:HA    | 1.93                     | 0.51              |
| 30:BH:73:ASN:ND2   | 30:BH:74:ALA:N     | 2.56                     | 0.51              |
| 31:BJ:39:LYS:C     | 31:BJ:41:LYS:H     | 2.17                     | 0.51              |
| 32:BK:78:ARG:O     | 37:BP:71:ARG:HB3   | 2.10                     | 0.51              |
| 33:BL:62:PRO:HB3   | 50:B3:29:ARG:NH2   | 2.25                     | 0.51              |
| 34:BM:20:LEU:HB2   | 34:BM:38:ARG:HD3   | 1.93                     | 0.51              |
| 35:BN:38:LEU:HB2   | 35:BN:109:PRO:CG   | 2.41                     | 0.51              |
| 36:BO:53:THR:O     | 36:BO:62:LEU:HD23  | 2.10                     | 0.51              |
| 37:BP:77:SER:HB2   | 37:BP:78:PRO:HD3   | 1.92                     | 0.51              |
| 37:BP:112:ARG:HH11 | 37:BP:112:ARG:N    | 2.08                     | 0.51              |
| 38:BQ:61:ILE:O     | 38:BQ:65:ASN:HB3   | 2.11                     | 0.51              |
| 41:BT:30:ILE:HG22  | 41:BT:85:VAL:HG22  | 1.92                     | 0.51              |
| 43:BW:44:PHE:HB3   | 43:BW:76:ARG:HA    | 1.92                     | 0.51              |
| 43:BW:66:VAL:CG1   | 43:BW:67:LYS:H     | 2.15                     | 0.51              |
| 46:BZ:5:ILE:HB     | 46:BZ:51:VAL:HG12  | 1.93                     | 0.51              |
| 52:BI:79:LEU:HD23  | 52:BI:108:ILE:CD1  | 2.41                     | 0.51              |
| 1:CA:423:G:H2'     | 1:CA:424:G:O4'     | 2.11                     | 0.51              |
| 1:CA:531:U:H5'     | 1:CA:531:U:H6      | 1.75                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:697:U:H2'     | 1:CA:698:G:H5'    | 1.93                     | 0.51              |
| 1:CA:1021:A:H2'    | 1:CA:1022:A:C1'   | 2.41                     | 0.51              |
| 1:CA:1085:U:H3'    | 1:CA:1086:U:C5    | 2.45                     | 0.51              |
| 1:CA:1325:C:O2'    | 1:CA:1326:U:H5'   | 2.10                     | 0.51              |
| 2:CC:85:LYS:HG3    | 2:CC:86:LEU:N     | 2.24                     | 0.51              |
| 3:CD:197:HIS:O     | 3:CD:201:GLU:HG3  | 2.10                     | 0.51              |
| 14:CO:48:ASP:CG    | 14:CO:51:SER:HB2  | 2.35                     | 0.51              |
| 19:CT:68:LYS:HB2   | 19:CT:70:LYS:HD3  | 1.93                     | 0.51              |
| 23:DB:274:C:H2'    | 23:DB:275:C:H6    | 1.76                     | 0.51              |
| 23:DB:576:U:H2'    | 23:DB:577:G:C8    | 2.45                     | 0.51              |
| 23:DB:686:U:H5''   | 49:D2:11:LYS:HE3  | 1.92                     | 0.51              |
| 23:DB:1973:G:H2'   | 23:DB:1974:C:H6   | 1.75                     | 0.51              |
| 23:DB:2045:C:H5''  | 47:D0:14:MET:SD   | 2.50                     | 0.51              |
| 23:DB:2199:A:O2'   | 46:DZ:34:LEU:HD21 | 2.09                     | 0.51              |
| 23:DB:2466:C:O2    | 34:DM:118:LYS:HD3 | 2.09                     | 0.51              |
| 23:DB:2597:G:C5'   | 25:DC:239:PHE:HB2 | 2.39                     | 0.51              |
| 23:DB:2849:U:O4    | 37:DP:96:LEU:HD21 | 2.11                     | 0.51              |
| 26:DD:37:VAL:CB    | 26:DD:46:ARG:HB2  | 2.39                     | 0.51              |
| 27:DE:137:LYS:HA   | 27:DE:137:LYS:HZ3 | 1.73                     | 0.51              |
| 28:DF:13:LYS:CA    | 28:DF:16:MET:HB2  | 2.34                     | 0.51              |
| 29:DG:171:LYS:HE2  | 29:DG:174:LYS:HG3 | 1.92                     | 0.51              |
| 32:DK:2:ILE:HA     | 32:DK:33:ALA:H    | 1.75                     | 0.51              |
| 33:DL:132:ARG:HH12 | 33:DL:140:GLY:HA2 | 1.74                     | 0.51              |
| 44:DX:7:ARG:O      | 44:DX:7:ARG:HG3   | 2.11                     | 0.51              |
| 45:DY:43:ILE:HD13  | 45:DY:43:ILE:C    | 2.35                     | 0.51              |
| 1:AA:522:C:H41     | 11:AL:49:ARG:NH2  | 2.09                     | 0.51              |
| 1:AA:837:U:H2'     | 1:AA:838:G:H8     | 1.75                     | 0.51              |
| 1:AA:1272:G:H2'    | 1:AA:1273:C:C6    | 2.45                     | 0.51              |
| 3:AD:24:VAL:O      | 3:AD:25:ARG:C     | 2.53                     | 0.51              |
| 3:AD:100:VAL:CG1   | 3:AD:104:MET:HE3  | 2.41                     | 0.51              |
| 6:AG:64:ALA:HA     | 6:AG:127:ALA:HB2  | 1.92                     | 0.51              |
| 7:AH:6:ILE:CG2     | 7:AH:76:ARG:HH12  | 2.24                     | 0.51              |
| 10:AK:63:GLN:HB3   | 10:AK:94:SER:OG   | 2.11                     | 0.51              |
| 13:AN:45:LEU:HD23  | 13:AN:45:LEU:C    | 2.36                     | 0.51              |
| 14:AO:29:ALA:HA    | 14:AO:84:LEU:HD21 | 1.92                     | 0.51              |
| 15:AP:67:ILE:CG1   | 15:AP:71:VAL:HG13 | 2.41                     | 0.51              |
| 15:AP:73:ALA:O     | 15:AP:77:GLU:HG3  | 2.10                     | 0.51              |
| 23:BB:354:A:C3'    | 23:BB:355:U:H5''  | 2.40                     | 0.51              |
| 23:BB:1025:G:OP1   | 23:BB:1025:G:H8   | 1.94                     | 0.51              |
| 23:BB:1535:A:H3'   | 23:BB:1536:C:C6   | 2.46                     | 0.51              |
| 23:BB:1771:C:H2'   | 23:BB:1772:A:C8   | 2.45                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:2074:U:H2'   | 23:BB:2075:U:C6    | 2.46                     | 0.51              |
| 23:BB:2329:U:H2'   | 23:BB:2330:G:H8    | 1.74                     | 0.51              |
| 23:BB:2688:G:H1'   | 23:BB:2721:A:N6    | 2.25                     | 0.51              |
| 23:BB:2886:A:C8    | 47:B0:27:LEU:HD22  | 2.46                     | 0.51              |
| 24:BV:80:HIS:CD2   | 24:BV:83:LYS:HB2   | 2.45                     | 0.51              |
| 25:BC:141:HIS:ND1  | 25:BC:142:ASN:N    | 2.59                     | 0.51              |
| 25:BC:160:TYR:HA   | 25:BC:193:GLU:CG   | 2.41                     | 0.51              |
| 26:BD:15:PHE:HD2   | 26:BD:18:ASP:HB2   | 1.75                     | 0.51              |
| 28:BF:16:MET:HE1   | 28:BF:22:ASN:N     | 2.26                     | 0.51              |
| 29:BG:120:ILE:CG1  | 29:BG:140:ILE:HG22 | 2.40                     | 0.51              |
| 33:BL:77:ILE:HA    | 33:BL:101:ILE:HD13 | 1.93                     | 0.51              |
| 33:BL:78:ARG:HH21  | 33:BL:82:LEU:HD23  | 1.74                     | 0.51              |
| 34:BM:9:PHE:CG     | 34:BM:10:ARG:N     | 2.79                     | 0.51              |
| 35:BN:29:VAL:HG13  | 35:BN:83:LEU:HD13  | 1.93                     | 0.51              |
| 41:BT:50:LEU:HD22  | 41:BT:50:LEU:N     | 2.26                     | 0.51              |
| 42:BU:42:LYS:O     | 42:BU:57:ILE:HG13  | 2.11                     | 0.51              |
| 42:BU:94:PHE:CZ    | 42:BU:100:GLU:HA   | 2.46                     | 0.51              |
| 46:BZ:58:ASP:CG    | 46:BZ:63:ARG:HH11  | 2.19                     | 0.51              |
| 52:BI:18:ASN:N     | 52:BI:19:PRO:CD    | 2.74                     | 0.51              |
| 1:CA:488:C:H2'     | 1:CA:489:C:H6      | 1.76                     | 0.51              |
| 1:CA:767:A:H2'     | 1:CA:768:A:C8      | 2.46                     | 0.51              |
| 1:CA:1004:A:H3'    | 1:CA:1005:A:H8     | 1.75                     | 0.51              |
| 3:CD:94:GLU:HA     | 3:CD:99:ASN:ND2    | 2.26                     | 0.51              |
| 8:CI:33:SER:HB2    | 8:CI:36:GLN:HG2    | 1.92                     | 0.51              |
| 16:CQ:16:MET:HB3   | 16:CQ:19:SER:HB2   | 1.92                     | 0.51              |
| 16:CQ:80:LYS:H     | 16:CQ:80:LYS:HD2   | 1.76                     | 0.51              |
| 20:CB:34:ARG:HE    | 20:CB:39:ILE:HG13  | 1.74                     | 0.51              |
| 23:DB:718:A:H3'    | 23:DB:719:C:H6     | 1.76                     | 0.51              |
| 23:DB:862:G:H2'    | 23:DB:863:A:O4'    | 2.11                     | 0.51              |
| 23:DB:866:A:H61    | 23:DB:913:U:C1'    | 2.24                     | 0.51              |
| 23:DB:2373:G:H2'   | 23:DB:2374:C:C6    | 2.45                     | 0.51              |
| 25:DC:257:ARG:HA   | 25:DC:261:ARG:NE   | 2.26                     | 0.51              |
| 27:DE:88:ARG:HB3   | 27:DE:89:PRO:CD    | 2.40                     | 0.51              |
| 27:DE:188:MET:SD   | 27:DE:190:ALA:HB2  | 2.51                     | 0.51              |
| 29:DG:172:GLU:OE1  | 51:D4:32:LYS:HB3   | 2.11                     | 0.51              |
| 30:DH:144:VAL:HG12 | 30:DH:145:ASN:H    | 1.76                     | 0.51              |
| 30:DH:147:VAL:HG12 | 30:DH:148:ALA:N    | 2.25                     | 0.51              |
| 31:DJ:81:ILE:HG12  | 31:DJ:83:GLY:H     | 1.76                     | 0.51              |
| 31:DJ:98:GLU:HG3   | 31:DJ:126:ALA:CB   | 2.41                     | 0.51              |
| 37:DP:59:THR:O     | 37:DP:60:VAL:HG13  | 2.10                     | 0.51              |
| 38:DQ:30:VAL:HG12  | 38:DQ:31:TYR:H     | 1.74                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:DQ:52:ARG:HG2   | 38:DQ:53:LYS:N     | 2.26                     | 0.51              |
| 39:DR:23:GLU:O     | 39:DR:96:VAL:HG21  | 2.11                     | 0.51              |
| 42:DU:59:GLU:HG3   | 42:DU:62:ALA:CB    | 2.38                     | 0.51              |
| 46:DZ:59:ARG:HD3   | 46:DZ:63:ARG:CD    | 2.41                     | 0.51              |
| 47:D0:41:HIS:CD2   | 47:D0:42:ILE:HG22  | 2.46                     | 0.51              |
| 50:D3:21:PHE:H     | 50:D3:48:MET:HB2   | 1.75                     | 0.51              |
| 51:D4:23:ILE:HD13  | 51:D4:24:ARG:H     | 1.74                     | 0.51              |
| 1:AA:132:C:H5''    | 19:AT:68:LYS:CD    | 2.40                     | 0.51              |
| 1:AA:488:C:H2'     | 1:AA:489:C:H6      | 1.76                     | 0.51              |
| 1:AA:1422:G:O2'    | 1:AA:1423:G:H5'    | 2.11                     | 0.51              |
| 5:AF:47:LEU:HD13   | 5:AF:51:ILE:HG22   | 1.92                     | 0.51              |
| 11:AL:79:ILE:C     | 11:AL:79:ILE:HD12  | 2.35                     | 0.51              |
| 13:AN:10:VAL:HG12  | 13:AN:11:LYS:NZ    | 2.26                     | 0.51              |
| 23:BB:10:A:O2'     | 23:BB:11:C:H5'     | 2.11                     | 0.51              |
| 23:BB:350:G:H2'    | 23:BB:351:C:C6     | 2.45                     | 0.51              |
| 23:BB:496:G:H2'    | 23:BB:497:A:O4'    | 2.10                     | 0.51              |
| 23:BB:1913:A:C1'   | 23:BB:1914:C:OP1   | 2.56                     | 0.51              |
| 23:BB:2060:A:H62   | 27:BE:69:ARG:HH21  | 1.57                     | 0.51              |
| 23:BB:2464:G:H2'   | 23:BB:2465:C:H6    | 1.75                     | 0.51              |
| 23:BB:2680:U:H5'   | 26:BD:194:PRO:HA   | 1.92                     | 0.51              |
| 23:BB:2756:U:OP2   | 51:B4:19:ARG:HD3   | 2.10                     | 0.51              |
| 23:BB:2849:U:H4'   | 23:BB:2868:A:C2    | 2.46                     | 0.51              |
| 23:BB:2877:G:O2'   | 23:BB:2878:U:H5'   | 2.11                     | 0.51              |
| 25:BC:160:TYR:O    | 25:BC:161:VAL:HG23 | 2.11                     | 0.51              |
| 27:BE:27:LEU:C     | 27:BE:27:LEU:HD13  | 2.36                     | 0.51              |
| 27:BE:84:THR:HG23  | 27:BE:85:PHE:N     | 2.26                     | 0.51              |
| 27:BE:105:LEU:HD22 | 27:BE:177:PRO:CG   | 2.40                     | 0.51              |
| 28:BF:90:LEU:HD23  | 28:BF:94:ARG:HG2   | 1.93                     | 0.51              |
| 31:BJ:13:ARG:HG3   | 31:BJ:13:ARG:NH1   | 2.22                     | 0.51              |
| 31:BJ:100:VAL:O    | 31:BJ:102:GLU:N    | 2.44                     | 0.51              |
| 32:BK:7:MET:HE1    | 32:BK:20:MET:HB2   | 1.93                     | 0.51              |
| 32:BK:76:VAL:O     | 37:BP:73:PHE:HA    | 2.11                     | 0.51              |
| 36:BO:68:LYS:H     | 36:BO:68:LYS:CD    | 2.23                     | 0.51              |
| 38:BQ:92:LYS:O     | 38:BQ:94:LEU:HD13  | 2.11                     | 0.51              |
| 40:BS:71:VAL:HG12  | 40:BS:71:VAL:O     | 2.11                     | 0.51              |
| 46:BZ:15:SER:HB3   | 46:BZ:23:LYS:CE    | 2.41                     | 0.51              |
| 48:B1:7:LYS:HD2    | 48:B1:8:ILE:O      | 2.11                     | 0.51              |
| 49:B2:10:LEU:O     | 49:B2:10:LEU:HD23  | 2.11                     | 0.51              |
| 50:B3:24:LYS:HA    | 50:B3:45:PRO:CB    | 2.35                     | 0.51              |
| 51:B4:22:VAL:HG21  | 51:B4:24:ARG:HH21  | 1.76                     | 0.51              |
| 1:CA:212:G:H2'     | 1:CA:213:G:C8      | 2.46                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:451:A:C5'     | 15:CP:70:ARG:HH22  | 2.17                     | 0.51              |
| 1:CA:1007:U:H2'    | 1:CA:1008:U:H6     | 1.75                     | 0.51              |
| 1:CA:1049:U:O2'    | 1:CA:1050:G:P      | 2.68                     | 0.51              |
| 1:CA:1262:C:H2'    | 1:CA:1263:C:C6     | 2.46                     | 0.51              |
| 1:CA:1306:A:H61    | 1:CA:1331:G:C1'    | 2.18                     | 0.51              |
| 1:CA:1369:C:H2'    | 1:CA:1370:G:C8     | 2.46                     | 0.51              |
| 1:CA:1391:U:H2'    | 1:CA:1392:G:H8     | 1.74                     | 0.51              |
| 2:CC:189:HIS:CD2   | 2:CC:194:VAL:HG22  | 2.45                     | 0.51              |
| 5:CF:38:ARG:HH21   | 5:CF:63:ASN:CG     | 2.18                     | 0.51              |
| 14:CO:35:ILE:O     | 14:CO:39:GLN:HG2   | 2.11                     | 0.51              |
| 15:CP:57:ILE:O     | 15:CP:61:VAL:HG23  | 2.11                     | 0.51              |
| 16:CQ:74:LEU:C     | 16:CQ:74:LEU:HD13  | 2.36                     | 0.51              |
| 18:CS:26:ASP:OD2   | 18:CS:46:LEU:HA    | 2.11                     | 0.51              |
| 23:DB:327:G:O2'    | 23:DB:328:U:H5'    | 2.11                     | 0.51              |
| 23:DB:630:G:H1     | 33:DL:69:ARG:NH1   | 2.09                     | 0.51              |
| 23:DB:877:A:H61    | 23:DB:898:C:H2'    | 1.74                     | 0.51              |
| 23:DB:956:G:N2     | 23:DB:959:A:H3'    | 2.25                     | 0.51              |
| 23:DB:1005:C:H2'   | 23:DB:1006:C:C6    | 2.46                     | 0.51              |
| 23:DB:1535:A:H3'   | 23:DB:1536:C:C6    | 2.46                     | 0.51              |
| 23:DB:1654:A:H4'   | 35:DN:1:MET:O      | 2.11                     | 0.51              |
| 23:DB:1717:A:H2'   | 23:DB:1718:G:O4'   | 2.10                     | 0.51              |
| 23:DB:1864:U:OP1   | 23:DB:2410:G:O2'   | 2.22                     | 0.51              |
| 23:DB:2291:U:H2'   | 23:DB:2292:U:H6    | 1.71                     | 0.51              |
| 23:DB:2393:U:H5'   | 33:DL:61:LEU:O     | 2.10                     | 0.51              |
| 23:DB:2515:C:O2'   | 23:DB:2516:A:H5'   | 2.11                     | 0.51              |
| 23:DB:2820:A:C5    | 26:DD:197:THR:HB   | 2.45                     | 0.51              |
| 26:DD:5:VAL:CG2    | 26:DD:28:GLU:HA    | 2.40                     | 0.51              |
| 27:DE:116:ASP:CG   | 27:DE:185:LYS:HE2  | 2.36                     | 0.51              |
| 27:DE:146:VAL:HG11 | 27:DE:184:ASP:OD1  | 2.11                     | 0.51              |
| 28:DF:91:ARG:C     | 28:DF:95:MET:HE2   | 2.36                     | 0.51              |
| 28:DF:163:GLU:HA   | 28:DF:166:ARG:CD   | 2.41                     | 0.51              |
| 29:DG:148:ARG:HH21 | 29:DG:153:PRO:HD2  | 1.76                     | 0.51              |
| 29:DG:172:GLU:O    | 29:DG:173:ALA:C    | 2.54                     | 0.51              |
| 32:DK:112:PHE:O    | 32:DK:114:LYS:N    | 2.43                     | 0.51              |
| 33:DL:14:LYS:HD2   | 33:DL:15:ALA:N     | 2.26                     | 0.51              |
| 33:DL:19:LEU:N     | 33:DL:19:LEU:HD13  | 2.25                     | 0.51              |
| 36:DO:86:GLY:O     | 36:DO:87:ILE:HD13  | 2.10                     | 0.51              |
| 38:DQ:82:LEU:HD11  | 38:DQ:108:LEU:HD11 | 1.92                     | 0.51              |
| 39:DR:33:VAL:H     | 39:DR:35:PHE:HD2   | 1.59                     | 0.51              |
| 42:DU:41:VAL:O     | 42:DU:42:LYS:HB2   | 2.10                     | 0.51              |
| 43:DW:20:LEU:HD11  | 43:DW:31:LEU:HB2   | 1.92                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:DX:28:LEU:HD13  | 44:DX:42:LEU:HD11  | 1.93                     | 0.51              |
| 45:DY:15:ARG:HD2   | 45:DY:53:MET:SD    | 2.51                     | 0.51              |
| 50:D3:2:LYS:HZ2    | 50:D3:2:LYS:CB     | 2.24                     | 0.51              |
| 51:D4:25:VAL:O     | 51:D4:35:GLN:HB2   | 2.10                     | 0.51              |
| 52:DI:79:LEU:HD12  | 52:DI:135:MET:SD   | 2.51                     | 0.51              |
| 1:AA:394:G:H2'     | 1:AA:395:C:C6      | 2.45                     | 0.51              |
| 1:AA:1101:A:N7     | 20:AB:170:ILE:HD12 | 2.25                     | 0.51              |
| 2:AC:42:LEU:O      | 2:AC:46:LEU:HB2    | 2.11                     | 0.51              |
| 11:AL:90:PRO:C     | 11:AL:92:VAL:H     | 2.18                     | 0.51              |
| 17:AR:22:TYR:HB2   | 17:AR:61:ALA:HB2   | 1.92                     | 0.51              |
| 20:AB:187:ASP:CG   | 20:AB:188:THR:N    | 2.69                     | 0.51              |
| 23:BB:55:G:H2'     | 23:BB:56:A:H8      | 1.76                     | 0.51              |
| 23:BB:320:A:H2'    | 27:BE:131:THR:HG21 | 1.92                     | 0.51              |
| 23:BB:1315:C:H2'   | 23:BB:1316:U:C6    | 2.46                     | 0.51              |
| 23:BB:1663:G:O2'   | 23:BB:2686:G:H4'   | 2.11                     | 0.51              |
| 23:BB:1733:G:H2'   | 23:BB:1734:G:C8    | 2.45                     | 0.51              |
| 23:BB:2364:C:H2'   | 23:BB:2365:G:O4'   | 2.10                     | 0.51              |
| 23:BB:2666:C:O4'   | 23:BB:2666:C:O2    | 2.24                     | 0.51              |
| 25:BC:45:ASN:O     | 25:BC:46:GLY:C     | 2.54                     | 0.51              |
| 26:BD:29:VAL:HG23  | 26:BD:51:THR:HG21  | 1.93                     | 0.51              |
| 26:BD:100:LEU:C    | 26:BD:102:ALA:H    | 2.19                     | 0.51              |
| 27:BE:169:VAL:HG12 | 27:BE:171:ASP:OD1  | 2.11                     | 0.51              |
| 30:BH:73:ASN:C     | 30:BH:75:LEU:H     | 2.19                     | 0.51              |
| 38:BQ:92:LYS:HA    | 38:BQ:95:ALA:CB    | 2.40                     | 0.51              |
| 38:BQ:92:LYS:HD3   | 38:BQ:93:ILE:HG22  | 1.92                     | 0.51              |
| 38:BQ:103:VAL:O    | 38:BQ:106:THR:HG22 | 2.11                     | 0.51              |
| 39:BR:40:MET:HA    | 39:BR:54:VAL:HG11  | 1.93                     | 0.51              |
| 42:BU:69:VAL:HG13  | 42:BU:77:GLY:H     | 1.75                     | 0.51              |
| 46:BZ:35:ASP:C     | 46:BZ:42:PRO:HB3   | 2.35                     | 0.51              |
| 46:BZ:59:ARG:HH21  | 46:BZ:62:LYS:NZ    | 2.09                     | 0.51              |
| 47:B0:35:GLU:CG    | 47:B0:36:LYS:N     | 2.73                     | 0.51              |
| 47:B0:45:ASP:HB2   | 47:B0:47:TYR:CD1   | 2.46                     | 0.51              |
| 49:B2:21:ARG:HB3   | 49:B2:31:LEU:HD21  | 1.91                     | 0.51              |
| 51:B4:9:LYS:O      | 51:B4:25:VAL:HG13  | 2.11                     | 0.51              |
| 52:BI:27:LEU:HB2   | 52:BI:32:VAL:HG21  | 1.92                     | 0.51              |
| 1:CA:402:G:H2'     | 1:CA:403:C:H6      | 1.75                     | 0.51              |
| 1:CA:499:A:C2      | 1:CA:546:A:N3      | 2.79                     | 0.51              |
| 1:CA:538:G:P       | 11:CL:111:GLN:HB2  | 2.51                     | 0.51              |
| 1:CA:769:G:O2'     | 1:CA:770:C:H5'     | 2.11                     | 0.51              |
| 1:CA:1041:G:H2'    | 1:CA:1042:A:C8     | 2.44                     | 0.51              |
| 1:CA:1238:A:C2     | 1:CA:1241:G:N3     | 2.79                     | 0.51              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:1287:A:O2'    | 1:CA:1288:A:H5'   | 2.11                     | 0.51              |
| 3:CD:75:TYR:HE1    | 3:CD:200:VAL:HG23 | 1.75                     | 0.51              |
| 3:CD:89:LEU:HA     | 3:CD:92:LEU:HB2   | 1.93                     | 0.51              |
| 5:CF:5:GLU:HA      | 5:CF:63:ASN:HA    | 1.92                     | 0.51              |
| 5:CF:53:LYS:HE2    | 5:CF:54:LEU:HD23  | 1.92                     | 0.51              |
| 5:CF:54:LEU:HD13   | 5:CF:55:HIS:H     | 1.76                     | 0.51              |
| 8:CI:51:LEU:CB     | 8:CI:56:MET:HG2   | 2.38                     | 0.51              |
| 12:CM:106:ARG:NH1  | 12:CM:109:LYS:HD2 | 2.26                     | 0.51              |
| 20:CB:113:LEU:HD23 | 20:CB:113:LEU:C   | 2.36                     | 0.51              |
| 23:DB:105:C:H2'    | 23:DB:106:C:H6    | 1.76                     | 0.51              |
| 23:DB:175:G:H2'    | 23:DB:176:A:H8    | 1.74                     | 0.51              |
| 23:DB:532:A:H5''   | 38:DQ:27:ARG:HH12 | 1.76                     | 0.51              |
| 23:DB:633:A:O5'    | 23:DB:633:A:C8    | 2.57                     | 0.51              |
| 23:DB:642:U:H2'    | 23:DB:644:A:OP2   | 2.10                     | 0.51              |
| 23:DB:1274:A:N3    | 23:DB:1297:C:H1'  | 2.25                     | 0.51              |
| 23:DB:1367:A:H2'   | 23:DB:1368:G:H5'  | 1.93                     | 0.51              |
| 23:DB:2017:U:H4'   | 47:D0:4:GLN:O     | 2.11                     | 0.51              |
| 23:DB:2278:A:N6    | 43:DW:10:ARG:HB2  | 2.25                     | 0.51              |
| 23:DB:2293:G:P     | 36:DO:13:ARG:HH22 | 2.33                     | 0.51              |
| 23:DB:2581:G:OP2   | 23:DB:2581:G:N2   | 2.43                     | 0.51              |
| 26:DD:204:LYS:HB3  | 26:DD:205:PRO:CD  | 2.30                     | 0.51              |
| 27:DE:116:ASP:C    | 27:DE:117:ARG:HD2 | 2.36                     | 0.51              |
| 31:DJ:15:TRP:CE3   | 31:DJ:138:GLN:HB2 | 2.45                     | 0.51              |
| 33:DL:41:ARG:CZ    | 33:DL:41:ARG:HA   | 2.41                     | 0.51              |
| 34:DM:131:VAL:CG2  | 34:DM:133:LYS:HB3 | 2.40                     | 0.51              |
| 36:DO:35:ILE:HG21  | 36:DO:74:VAL:HG21 | 1.93                     | 0.51              |
| 40:DS:68:ASP:HB2   | 40:DS:69:LEU:HD22 | 1.93                     | 0.51              |
| 46:DZ:50:ASP:HA    | 46:DZ:53:THR:HG22 | 1.92                     | 0.51              |
| 49:D2:16:HIS:NE2   | 49:D2:44:VAL:HG12 | 2.26                     | 0.51              |
| 49:D2:19:ARG:HD3   | 49:D2:19:ARG:C    | 2.35                     | 0.51              |
| 50:D3:4:LYS:CE     | 50:D3:61:LEU:HD13 | 2.41                     | 0.51              |
| 50:D3:12:ARG:HD2   | 50:D3:24:LYS:O    | 2.10                     | 0.51              |
| 52:DI:23:VAL:HG12  | 52:DI:24:GLY:N    | 2.26                     | 0.51              |
| 1:AA:539:A:H2'     | 1:AA:540:G:H8     | 1.74                     | 0.51              |
| 1:AA:767:A:H2'     | 1:AA:768:A:C8     | 2.46                     | 0.51              |
| 1:AA:1122:U:H2'    | 1:AA:1123:U:C6    | 2.46                     | 0.51              |
| 1:AA:1150:A:H1'    | 1:AA:1280:A:N6    | 2.26                     | 0.51              |
| 1:AA:1202:U:C2'    | 1:AA:1203:C:H5'   | 2.41                     | 0.51              |
| 1:AA:1338:G:H2'    | 1:AA:1339:A:C8    | 2.45                     | 0.51              |
| 1:AA:1486:G:H2'    | 1:AA:1487:G:C8    | 2.46                     | 0.51              |
| 2:AC:146:LYS:HB2   | 2:AC:146:LYS:NZ   | 2.25                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:AC:184:ASN:HD22  | 2:AC:185:THR:N     | 2.08                     | 0.51              |
| 8:AI:10:ARG:HA     | 8:AI:77:ALA:HB1    | 1.92                     | 0.51              |
| 8:AI:113:LYS:HG2   | 8:AI:114:LYS:N     | 2.26                     | 0.51              |
| 10:AK:110:THR:CG2  | 21:AU:4:LYS:HD2    | 2.39                     | 0.51              |
| 20:AB:67:LEU:HD21  | 20:AB:157:PRO:CG   | 2.41                     | 0.51              |
| 20:AB:164:ASP:CG   | 20:AB:203:ASP:HB2  | 2.36                     | 0.51              |
| 23:BB:37:C:C2      | 27:BE:46:GLN:OE1   | 2.64                     | 0.51              |
| 23:BB:538:A:O2'    | 23:BB:539:G:H5'    | 2.10                     | 0.51              |
| 23:BB:854:C:O2'    | 23:BB:855:G:H5'    | 2.11                     | 0.51              |
| 23:BB:1269:A:H2'   | 23:BB:1270:C:C6    | 2.46                     | 0.51              |
| 23:BB:1360:G:H2'   | 23:BB:1361:G:C5'   | 2.41                     | 0.51              |
| 23:BB:2076:U:O4'   | 23:BB:2076:U:O2    | 2.29                     | 0.51              |
| 23:BB:2314:A:H5'   | 28:BF:34:THR:HG21  | 1.92                     | 0.51              |
| 23:BB:2520:C:C6    | 23:BB:2567:G:H1'   | 2.46                     | 0.51              |
| 23:BB:2653:U:H3'   | 23:BB:2654:A:H2'   | 1.92                     | 0.51              |
| 25:BC:248:GLY:HA3  | 25:BC:252:LYS:HE3  | 1.91                     | 0.51              |
| 27:BE:78:TRP:HE3   | 27:BE:78:TRP:N     | 2.09                     | 0.51              |
| 27:BE:119:ILE:HG23 | 27:BE:189:THR:O    | 2.11                     | 0.51              |
| 28:BF:33:ILE:HG13  | 28:BF:34:THR:H     | 1.76                     | 0.51              |
| 28:BF:108:PRO:HB3  | 28:BF:113:PHE:CD2  | 2.46                     | 0.51              |
| 28:BF:121:PHE:CZ   | 28:BF:169:LEU:HD12 | 2.46                     | 0.51              |
| 36:BO:25:ARG:HD3   | 36:BO:40:ILE:HD11  | 1.92                     | 0.51              |
| 37:BP:23:ASP:OD2   | 37:BP:93:LYS:HG2   | 2.10                     | 0.51              |
| 41:BT:43:ILE:O     | 41:BT:47:VAL:HG23  | 2.11                     | 0.51              |
| 41:BT:96:VAL:HG22  | 41:BT:97:GLY:H     | 1.75                     | 0.51              |
| 1:CA:35:G:H2'      | 1:CA:36:C:C6       | 2.46                     | 0.51              |
| 1:CA:53:A:C2       | 1:CA:54:C:H1'      | 2.46                     | 0.51              |
| 1:CA:205:A:H2'     | 1:CA:206:C:C6      | 2.44                     | 0.51              |
| 1:CA:662:U:H2'     | 1:CA:663:A:H8      | 1.75                     | 0.51              |
| 4:CE:28:ARG:NH2    | 4:CE:30:PHE:HB3    | 2.26                     | 0.51              |
| 4:CE:156:ARG:HH22  | 7:CH:100:ILE:HG23  | 1.75                     | 0.51              |
| 10:CK:14:GLN:HA    | 10:CK:77:GLY:HA3   | 1.92                     | 0.51              |
| 12:CM:6:ILE:HD12   | 12:CM:6:ILE:N      | 2.26                     | 0.51              |
| 12:CM:50:GLY:O     | 12:CM:54:THR:HG23  | 2.11                     | 0.51              |
| 23:DB:361:G:O2'    | 23:DB:362:A:H5'    | 2.11                     | 0.51              |
| 23:DB:545:U:H3'    | 23:DB:546:U:C5'    | 2.40                     | 0.51              |
| 23:DB:910:A:H62    | 34:DM:15:GLY:HA3   | 1.75                     | 0.51              |
| 23:DB:919:U:H2'    | 23:DB:920:A:H8     | 1.69                     | 0.51              |
| 23:DB:1196:C:H2'   | 23:DB:1197:G:H8    | 1.75                     | 0.51              |
| 23:DB:1248:G:P     | 27:DE:44:ARG:HH22  | 2.34                     | 0.51              |
| 23:DB:1309:G:OP1   | 49:D2:9:VAL:HG22   | 2.11                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 23:DB:1828:G:O6   | 25:DC:219:VAL:HG11  | 2.11                     | 0.51              |
| 23:DB:2241:A:O2'  | 23:DB:2242:G:H5'    | 2.10                     | 0.51              |
| 23:DB:2669:G:H2'  | 23:DB:2670:A:H8     | 1.76                     | 0.51              |
| 23:DB:2821:A:H2'  | 23:DB:2822:G:C8     | 2.46                     | 0.51              |
| 24:DV:21:ARG:HH21 | 24:DV:88:HIS:N      | 2.08                     | 0.51              |
| 25:DC:48:ILE:CG2  | 25:DC:49:THR:H      | 2.06                     | 0.51              |
| 26:DD:5:VAL:HG12  | 26:DD:6:GLY:H       | 1.75                     | 0.51              |
| 27:DE:23:PHE:C    | 27:DE:110:SER:HB2   | 2.36                     | 0.51              |
| 27:DE:85:PHE:O    | 27:DE:86:ALA:CB     | 2.59                     | 0.51              |
| 29:DG:3:VAL:HG22  | 29:DG:4:ALA:N       | 2.25                     | 0.51              |
| 29:DG:55:ASP:CG   | 29:DG:56:GLY:N      | 2.69                     | 0.51              |
| 30:DH:68:ARG:HD3  | 30:DH:71:LYS:HB2    | 1.92                     | 0.51              |
| 31:DJ:123:LYS:N   | 31:DJ:123:LYS:HD2   | 2.25                     | 0.51              |
| 31:DJ:130:HIS:O   | 31:DJ:131:ASN:C     | 2.54                     | 0.51              |
| 33:DL:57:LEU:O    | 33:DL:58:TYR:HB2    | 2.10                     | 0.51              |
| 52:DI:59:THR:O    | 52:DI:59:THR:HG23   | 2.09                     | 0.51              |
| 1:AA:80:A:N3      | 1:AA:81:A:H1'       | 2.26                     | 0.50              |
| 1:AA:370:C:H2'    | 1:AA:371:A:C8       | 2.46                     | 0.50              |
| 1:AA:692:U:H5     | 10:AK:27:ASN:HD22   | 1.58                     | 0.50              |
| 1:AA:712:A:O2'    | 1:AA:713:G:H5'      | 2.12                     | 0.50              |
| 1:AA:1498:U:H3'   | 53:AA:1601:KSG:HN12 | 1.77                     | 0.50              |
| 4:AE:55:VAL:N     | 4:AE:56:PRO:HD2     | 2.26                     | 0.50              |
| 5:AF:7:VAL:HG11   | 17:AR:64:LEU:HD21   | 1.92                     | 0.50              |
| 9:AJ:30:LYS:O     | 9:AJ:30:LYS:HD2     | 2.11                     | 0.50              |
| 9:AJ:73:LEU:CD1   | 9:AJ:75:ASP:HB3     | 2.42                     | 0.50              |
| 15:AP:36:VAL:O    | 15:AP:36:VAL:HG13   | 2.12                     | 0.50              |
| 16:AQ:46:HIS:HB2  | 16:AQ:70:LYS:HE3    | 1.93                     | 0.50              |
| 23:BB:1739:A:H2'  | 23:BB:1740:G:H8     | 1.74                     | 0.50              |
| 23:BB:1797:G:H5'  | 25:BC:251:THR:HA    | 1.93                     | 0.50              |
| 23:BB:2195:U:H2'  | 23:BB:2196:C:C6     | 2.46                     | 0.50              |
| 24:BV:53:LYS:HE3  | 24:BV:55:GLU:HG3    | 1.92                     | 0.50              |
| 25:BC:160:TYR:HE2 | 25:BC:194:VAL:HA    | 1.76                     | 0.50              |
| 26:BD:83:ARG:HH11 | 26:BD:83:ARG:HG2    | 1.76                     | 0.50              |
| 26:BD:129:THR:O   | 26:BD:130:GLN:HB2   | 2.10                     | 0.50              |
| 26:BD:165:MET:HE3 | 26:BD:166:GLY:O     | 2.11                     | 0.50              |
| 27:BE:3:LEU:HA    | 27:BE:117:ARG:CZ    | 2.41                     | 0.50              |
| 28:BF:118:ALA:HB2 | 28:BF:177:ARG:NH1   | 2.25                     | 0.50              |
| 29:BG:63:GLN:HG3  | 29:BG:64:ALA:N      | 2.26                     | 0.50              |
| 30:BH:57:LYS:HA   | 30:BH:57:LYS:HE3    | 1.93                     | 0.50              |
| 32:BK:84:CYS:O    | 32:BK:85:VAL:HB     | 2.10                     | 0.50              |
| 34:BM:73:ILE:O    | 34:BM:74:THR:HB     | 2.11                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:BQ:61:ILE:HB    | 38:BQ:75:TYR:CE2   | 2.46                     | 0.50              |
| 39:BR:37:GLU:HG3   | 39:BR:38:VAL:N     | 2.26                     | 0.50              |
| 41:BT:6:ARG:C      | 41:BT:8:LEU:H      | 2.18                     | 0.50              |
| 41:BT:58:VAL:HG12  | 41:BT:59:ASN:N     | 2.26                     | 0.50              |
| 43:BW:45:HIS:HA    | 43:BW:75:ASN:HB2   | 1.91                     | 0.50              |
| 1:CA:176:C:H2'     | 1:CA:177:G:N3      | 2.26                     | 0.50              |
| 1:CA:865:A:C2      | 1:CA:918:A:H4'     | 2.46                     | 0.50              |
| 1:CA:1228:C:C5'    | 12:CM:112:ARG:HB3  | 2.41                     | 0.50              |
| 1:CA:1251:A:O2'    | 1:CA:1370:G:H5'    | 2.12                     | 0.50              |
| 1:CA:1319:A:P      | 18:CS:4:LEU:HD21   | 2.51                     | 0.50              |
| 1:CA:1461:G:O2'    | 1:CA:1462:C:H5'    | 2.11                     | 0.50              |
| 8:CI:29:ILE:HG23   | 8:CI:29:ILE:O      | 2.11                     | 0.50              |
| 9:CJ:28:THR:HG22   | 9:CJ:86:ALA:HB1    | 1.92                     | 0.50              |
| 12:CM:23:GLY:N     | 12:CM:69:ARG:HH22  | 2.09                     | 0.50              |
| 12:CM:85:TYR:HA    | 12:CM:88:LEU:HD12  | 1.92                     | 0.50              |
| 14:CO:11:VAL:HG21  | 14:CO:21:THR:HG22  | 1.92                     | 0.50              |
| 15:CP:60:TRP:HB3   | 15:CP:65:ALA:HB2   | 1.92                     | 0.50              |
| 16:CQ:32:ILE:O     | 16:CQ:32:ILE:HG12  | 2.11                     | 0.50              |
| 18:CS:62:THR:HG23  | 18:CS:63:ASP:N     | 2.26                     | 0.50              |
| 22:DA:40:U:O2      | 22:DA:43:C:H5''    | 2.11                     | 0.50              |
| 23:DB:466:A:H2'    | 23:DB:467:G:H5'    | 1.92                     | 0.50              |
| 23:DB:1083:U:H2'   | 23:DB:1085:A:OP2   | 2.11                     | 0.50              |
| 23:DB:1091:G:O2'   | 23:DB:1092:C:H5'   | 2.11                     | 0.50              |
| 23:DB:1175:A:C3'   | 23:DB:1176:U:H5'   | 2.40                     | 0.50              |
| 23:DB:2313:C:H2'   | 23:DB:2314:A:H8    | 1.76                     | 0.50              |
| 23:DB:2360:G:H5'   | 33:DL:58:TYR:OH    | 2.11                     | 0.50              |
| 23:DB:2653:U:H3'   | 23:DB:2654:A:H2'   | 1.92                     | 0.50              |
| 24:DV:26:PHE:CE1   | 24:DV:42:LEU:HD12  | 2.46                     | 0.50              |
| 28:DF:36:ASN:O     | 28:DF:151:LEU:HD12 | 2.11                     | 0.50              |
| 31:DJ:81:ILE:HG12  | 31:DJ:82:GLY:N     | 2.24                     | 0.50              |
| 32:DK:11:ALA:C     | 32:DK:100:PHE:H    | 2.20                     | 0.50              |
| 33:DL:59:ARG:HH12  | 50:D3:58:ILE:HG21  | 1.75                     | 0.50              |
| 33:DL:103:ILE:HG13 | 33:DL:104:GLN:N    | 2.22                     | 0.50              |
| 35:DN:9:GLN:HE22   | 35:DN:39:PRO:HB3   | 1.75                     | 0.50              |
| 35:DN:102:PHE:CZ   | 35:DN:104:ALA:HB2  | 2.46                     | 0.50              |
| 36:DO:90:VAL:HG11  | 36:DO:116:GLN:O    | 2.10                     | 0.50              |
| 39:DR:69:GLY:H     | 39:DR:97:LYS:HB2   | 1.75                     | 0.50              |
| 43:DW:42:THR:HG21  | 43:DW:66:VAL:HG13  | 1.93                     | 0.50              |
| 43:DW:67:LYS:HZ2   | 43:DW:70:VAL:HB    | 1.75                     | 0.50              |
| 45:DY:26:LEU:C     | 45:DY:28:LEU:H     | 2.19                     | 0.50              |
| 46:DZ:32:LEU:N     | 46:DZ:32:LEU:HD22  | 2.26                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:DZ:55:GLY:O     | 46:DZ:60:PHE:N     | 2.44                     | 0.50              |
| 1:AA:53:A:C2       | 1:AA:54:C:H1'      | 2.46                     | 0.50              |
| 1:AA:402:G:H2'     | 1:AA:403:C:H6      | 1.75                     | 0.50              |
| 1:AA:505:G:H5'     | 1:AA:534:U:H2'     | 1.94                     | 0.50              |
| 1:AA:629:A:H2'     | 1:AA:630:A:O4'     | 2.11                     | 0.50              |
| 1:AA:1402:C:H2'    | 1:AA:1403:C:O4'    | 2.11                     | 0.50              |
| 2:AC:38:VAL:HG12   | 2:AC:93:ILE:CG2    | 2.42                     | 0.50              |
| 3:AD:170:LEU:HB2   | 3:AD:180:THR:O     | 2.11                     | 0.50              |
| 6:AG:119:LEU:HD13  | 6:AG:119:LEU:C     | 2.36                     | 0.50              |
| 8:AI:32:ARG:NH2    | 8:AI:36:GLN:HG2    | 2.26                     | 0.50              |
| 10:AK:113:THR:HG21 | 21:AU:28:LEU:HD21  | 1.93                     | 0.50              |
| 19:AT:60:GLN:CD    | 19:AT:60:GLN:H     | 2.19                     | 0.50              |
| 20:AB:139:GLU:HG2  | 20:AB:143:LEU:HG   | 1.92                     | 0.50              |
| 21:AU:3:ILE:HG12   | 21:AU:19:LYS:HB3   | 1.92                     | 0.50              |
| 23:BB:85:G:OP1     | 42:BU:5:ARG:HA     | 2.12                     | 0.50              |
| 23:BB:221:A:H2'    | 23:BB:266:G:N7     | 2.26                     | 0.50              |
| 23:BB:243:U:OP1    | 50:B3:4:LYS:HG2    | 2.11                     | 0.50              |
| 23:BB:256:A:H2'    | 23:BB:257:C:H6     | 1.77                     | 0.50              |
| 23:BB:557:C:H2'    | 23:BB:558:U:C6     | 2.46                     | 0.50              |
| 23:BB:841:G:O2'    | 23:BB:842:U:H5'    | 2.12                     | 0.50              |
| 23:BB:1439:A:N7    | 23:BB:1440:U:C2    | 2.79                     | 0.50              |
| 23:BB:1930:G:HO2'  | 23:BB:1931:U:H5    | 1.57                     | 0.50              |
| 23:BB:2515:C:O2'   | 23:BB:2516:A:H5'   | 2.11                     | 0.50              |
| 23:BB:2636:C:H2'   | 23:BB:2637:U:C6    | 2.46                     | 0.50              |
| 23:BB:2896:C:H2'   | 23:BB:2897:U:C6    | 2.46                     | 0.50              |
| 24:BV:21:ARG:HE    | 24:BV:87:GLN:HB3   | 1.75                     | 0.50              |
| 25:BC:44:ASN:HA    | 25:BC:49:THR:O     | 2.11                     | 0.50              |
| 25:BC:137:GLY:C    | 25:BC:139:THR:H    | 2.18                     | 0.50              |
| 25:BC:172:THR:O    | 25:BC:173:LEU:HB2  | 2.11                     | 0.50              |
| 25:BC:207:ALA:HA   | 25:BC:211:ARG:HB2  | 1.93                     | 0.50              |
| 26:BD:13:ARG:HB2   | 26:BD:21:SER:HB2   | 1.93                     | 0.50              |
| 26:BD:17:GLU:OE1   | 37:BP:32:VAL:HG11  | 2.12                     | 0.50              |
| 26:BD:87:GLY:O     | 26:BD:88:GLU:HB2   | 2.10                     | 0.50              |
| 26:BD:131:ASP:CG   | 26:BD:132:ALA:N    | 2.69                     | 0.50              |
| 27:BE:151:GLY:HA2  | 27:BE:171:ASP:HA   | 1.93                     | 0.50              |
| 28:BF:140:ILE:HG22 | 28:BF:142:TYR:H    | 1.76                     | 0.50              |
| 31:BJ:52:ASP:CG    | 31:BJ:53:TYR:H     | 2.19                     | 0.50              |
| 31:BJ:137:PRO:O    | 31:BJ:139:VAL:HG13 | 2.11                     | 0.50              |
| 33:BL:126:ARG:NH2  | 33:BL:131:ALA:CB   | 2.73                     | 0.50              |
| 37:BP:9:GLN:CD     | 37:BP:56:SER:HB2   | 2.36                     | 0.50              |
| 37:BP:57:ALA:C     | 37:BP:59:THR:H     | 2.19                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:BQ:22:GLY:HA2   | 38:BQ:28:SER:OG    | 2.10                     | 0.50              |
| 38:BQ:71:ASN:HD22  | 38:BQ:109:VAL:HG21 | 1.77                     | 0.50              |
| 38:BQ:84:LYS:O     | 38:BQ:85:ALA:HB2   | 2.12                     | 0.50              |
| 39:BR:4:VAL:HG22   | 39:BR:5:PHE:N      | 2.26                     | 0.50              |
| 44:BX:59:GLU:C     | 44:BX:61:ALA:H     | 2.19                     | 0.50              |
| 50:B3:47:ALA:O     | 50:B3:48:MET:HG3   | 2.11                     | 0.50              |
| 1:CA:346:G:OP1     | 37:DP:43:GLU:HG3   | 2.11                     | 0.50              |
| 1:CA:676:A:O2'     | 1:CA:677:U:H5'     | 2.10                     | 0.50              |
| 1:CA:724:G:O2'     | 1:CA:725:G:H5'     | 2.11                     | 0.50              |
| 1:CA:908:A:H2'     | 1:CA:909:A:C8      | 2.46                     | 0.50              |
| 1:CA:1338:G:H2'    | 1:CA:1339:A:C8     | 2.46                     | 0.50              |
| 1:CA:1411:C:H2'    | 1:CA:1412:C:H6     | 1.77                     | 0.50              |
| 3:CD:71:PHE:HA     | 3:CD:74:TYR:HD2    | 1.75                     | 0.50              |
| 3:CD:81:LEU:HB2    | 3:CD:88:ASN:ND2    | 2.25                     | 0.50              |
| 4:CE:109:ALA:HB3   | 4:CE:135:VAL:CG1   | 2.41                     | 0.50              |
| 6:CG:56:SER:HB3    | 6:CG:59:GLU:HB2    | 1.92                     | 0.50              |
| 9:CJ:66:GLU:HB2    | 13:CN:98:ALA:CB    | 2.39                     | 0.50              |
| 10:CK:70:ALA:O     | 10:CK:74:LYS:HB2   | 2.10                     | 0.50              |
| 13:CN:17:ASP:C     | 13:CN:19:TYR:H     | 2.19                     | 0.50              |
| 16:CQ:46:HIS:HB3   | 16:CQ:73:THR:HG22  | 1.94                     | 0.50              |
| 17:CR:51:GLN:HE21  | 17:CR:54:LEU:HB2   | 1.76                     | 0.50              |
| 23:DB:401:A:O2'    | 23:DB:402:A:H5'    | 2.11                     | 0.50              |
| 23:DB:723:C:H2'    | 23:DB:724:U:C6     | 2.47                     | 0.50              |
| 23:DB:729:G:H4'    | 23:DB:763:G:H5'    | 1.92                     | 0.50              |
| 23:DB:1029:A:H2'   | 23:DB:1030:C:O4'   | 2.11                     | 0.50              |
| 23:DB:1211:C:O2'   | 23:DB:1212:G:P     | 2.69                     | 0.50              |
| 23:DB:1269:A:H2'   | 23:DB:1270:C:C6    | 2.46                     | 0.50              |
| 23:DB:1917:U:C2'   | 23:DB:1918:A:H5'   | 2.42                     | 0.50              |
| 23:DB:1939:U:H5'   | 23:DB:1939:U:H6    | 1.75                     | 0.50              |
| 23:DB:2076:U:O4'   | 23:DB:2076:U:O2    | 2.29                     | 0.50              |
| 23:DB:2107:G:H2'   | 23:DB:2108:A:C8    | 2.45                     | 0.50              |
| 23:DB:2514:U:H2'   | 23:DB:2515:C:C6    | 2.47                     | 0.50              |
| 23:DB:2899:A:H2'   | 23:DB:2900:A:H8    | 1.74                     | 0.50              |
| 24:DV:9:ARG:NE     | 24:DV:20:LEU:HD11  | 2.27                     | 0.50              |
| 26:DD:37:VAL:HG12  | 26:DD:44:GLY:O     | 2.10                     | 0.50              |
| 26:DD:116:LYS:HB3  | 35:DN:1:MET:HA     | 1.94                     | 0.50              |
| 29:DG:120:ILE:HD13 | 29:DG:140:ILE:HD13 | 1.93                     | 0.50              |
| 30:DH:72:ILE:HG22  | 30:DH:72:ILE:O     | 2.11                     | 0.50              |
| 33:DL:85:VAL:HG21  | 33:DL:96:LYS:HG3   | 1.94                     | 0.50              |
| 37:DP:28:LYS:O     | 37:DP:30:TRP:N     | 2.44                     | 0.50              |
| 43:DW:23:LYS:HG2   | 43:DW:57:THR:HA    | 1.92                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:D1:7:LYS:HG2   | 48:D1:26:LYS:N     | 2.26                     | 0.50              |
| 49:D2:43:THR:C    | 49:D2:44:VAL:HG22  | 2.36                     | 0.50              |
| 52:DI:52:LEU:HD22 | 52:DI:81:LYS:HD3   | 1.92                     | 0.50              |
| 1:AA:423:G:H2'    | 1:AA:424:G:O4'     | 2.10                     | 0.50              |
| 1:AA:685:G:O2'    | 1:AA:686:U:H5'     | 2.10                     | 0.50              |
| 3:AD:96:ARG:O     | 3:AD:100:VAL:HG23  | 2.11                     | 0.50              |
| 3:AD:197:HIS:O    | 3:AD:201:GLU:HG3   | 2.10                     | 0.50              |
| 4:AE:71:ILE:HG12  | 4:AE:72:ASN:N      | 2.27                     | 0.50              |
| 7:AH:40:LYS:HD2   | 7:AH:48:PHE:CE1    | 2.47                     | 0.50              |
| 7:AH:110:MET:HB3  | 7:AH:114:ALA:HB3   | 1.93                     | 0.50              |
| 8:AI:23:GLY:N     | 8:AI:60:LEU:HA     | 2.24                     | 0.50              |
| 8:AI:71:ILE:HD12  | 8:AI:71:ILE:N      | 2.23                     | 0.50              |
| 9:AJ:92:LEU:HD22  | 9:AJ:92:LEU:N      | 2.25                     | 0.50              |
| 13:AN:30:ILE:CG2  | 13:AN:41:TRP:HB2   | 2.37                     | 0.50              |
| 15:AP:57:ILE:O    | 15:AP:61:VAL:HG22  | 2.11                     | 0.50              |
| 16:AQ:35:LYS:O    | 16:AQ:37:ILE:HG13  | 2.11                     | 0.50              |
| 18:AS:29:PRO:HA   | 18:AS:47:THR:HB    | 1.94                     | 0.50              |
| 20:AB:184:ALA:HB3 | 20:AB:195:VAL:HG21 | 1.93                     | 0.50              |
| 22:BA:13:G:O2'    | 22:BA:15:A:H5''    | 2.11                     | 0.50              |
| 23:BB:137:U:H2'   | 23:BB:138:U:H5'    | 1.94                     | 0.50              |
| 23:BB:529:A:OP2   | 31:BJ:113:PRO:HD3  | 2.11                     | 0.50              |
| 23:BB:910:A:C8    | 34:BM:16:ARG:HB2   | 2.46                     | 0.50              |
| 23:BB:1038:G:H2'  | 23:BB:1039:A:H8    | 1.76                     | 0.50              |
| 23:BB:2514:U:H2'  | 23:BB:2515:C:C6    | 2.46                     | 0.50              |
| 23:BB:2630:G:H2'  | 23:BB:2631:G:H8    | 1.76                     | 0.50              |
| 23:BB:2682:A:O2'  | 23:BB:2683:C:H5'   | 2.11                     | 0.50              |
| 23:BB:2867:G:N3   | 23:BB:2867:G:C2'   | 2.73                     | 0.50              |
| 25:BC:260:LYS:C   | 25:BC:262:THR:N    | 2.70                     | 0.50              |
| 26:BD:135:GLY:C   | 26:BD:137:SER:N    | 2.69                     | 0.50              |
| 27:BE:46:GLN:O    | 27:BE:48:THR:N     | 2.44                     | 0.50              |
| 27:BE:165:HIS:O   | 27:BE:166:LYS:HG3  | 2.11                     | 0.50              |
| 28:BF:116:LEU:H   | 28:BF:176:PHE:HA   | 1.76                     | 0.50              |
| 29:BG:25:ILE:O    | 29:BG:25:ILE:HG23  | 2.11                     | 0.50              |
| 29:BG:85:LYS:HA   | 29:BG:130:ILE:O    | 2.11                     | 0.50              |
| 30:BH:68:ARG:HG3  | 30:BH:134:VAL:CG1  | 2.38                     | 0.50              |
| 30:BH:90:LEU:CD2  | 30:BH:146:VAL:HG11 | 2.41                     | 0.50              |
| 33:BL:56:PRO:C    | 33:BL:60:ARG:HB2   | 2.35                     | 0.50              |
| 33:BL:83:ALA:HB2  | 33:BL:120:VAL:HG23 | 1.94                     | 0.50              |
| 38:BQ:102:LYS:HG2 | 38:BQ:103:VAL:N    | 2.26                     | 0.50              |
| 39:BR:48:LYS:C    | 39:BR:49:ILE:HD13  | 2.36                     | 0.50              |
| 43:BW:24:ARG:HD2  | 43:BW:57:THR:O     | 2.12                     | 0.50              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 44:BX:11:VAL:HG22  | 44:BX:11:VAL:O    | 2.10                     | 0.50              |
| 44:BX:18:LEU:HD23  | 44:BX:18:LEU:H    | 1.76                     | 0.50              |
| 48:B1:10:LEU:HD21  | 48:B1:34:GLU:HG3  | 1.93                     | 0.50              |
| 52:BI:5:GLN:HG2    | 52:BI:6:ALA:H     | 1.74                     | 0.50              |
| 52:BI:138:VAL:HG12 | 52:BI:139:VAL:N   | 2.26                     | 0.50              |
| 1:CA:98:A:H2'      | 1:CA:99:C:H6      | 1.73                     | 0.50              |
| 1:CA:314:C:O2'     | 1:CA:315:A:H5'    | 2.11                     | 0.50              |
| 1:CA:706:A:H2      | 10:CK:40:ALA:HB2  | 1.75                     | 0.50              |
| 1:CA:783:C:O2'     | 1:CA:784:A:H5'    | 2.10                     | 0.50              |
| 1:CA:853:C:O2'     | 1:CA:854:U:H5'    | 2.12                     | 0.50              |
| 1:CA:1520:C:H2'    | 1:CA:1521:C:H6    | 1.74                     | 0.50              |
| 2:CC:127:VAL:HG23  | 2:CC:128:MET:N    | 2.26                     | 0.50              |
| 5:CF:39:LEU:O      | 5:CF:39:LEU:HD13  | 2.11                     | 0.50              |
| 6:CG:45:ALA:HB1    | 6:CG:120:ALA:HB2  | 1.93                     | 0.50              |
| 6:CG:96:ASN:HB3    | 6:CG:100:MET:HE3  | 1.93                     | 0.50              |
| 9:CJ:17:LEU:HD13   | 9:CJ:17:LEU:C     | 2.35                     | 0.50              |
| 11:CL:86:VAL:HG11  | 11:CL:89:LEU:HD23 | 1.93                     | 0.50              |
| 18:CS:38:THR:HA    | 18:CS:69:LYS:HA   | 1.93                     | 0.50              |
| 18:CS:44:ILE:HG23  | 18:CS:63:ASP:HB2  | 1.94                     | 0.50              |
| 23:DB:64:A:H5''    | 41:DT:76:ARG:HG3  | 1.94                     | 0.50              |
| 23:DB:633:A:H2'    | 23:DB:634:C:C5'   | 2.41                     | 0.50              |
| 23:DB:773:U:H5'    | 23:DB:774:G:OP2   | 2.11                     | 0.50              |
| 23:DB:850:U:H2'    | 23:DB:851:C:H6    | 1.76                     | 0.50              |
| 23:DB:1438:U:H5'   | 23:DB:1516:G:O2'  | 2.10                     | 0.50              |
| 23:DB:1655:A:H4'   | 26:DD:120:GLY:N   | 2.26                     | 0.50              |
| 23:DB:1916:A:H2'   | 23:DB:1917:U:O4'  | 2.11                     | 0.50              |
| 23:DB:2139:U:O2'   | 23:DB:2140:G:H5'  | 2.11                     | 0.50              |
| 23:DB:2471:A:O2'   | 23:DB:2472:G:C8   | 2.54                     | 0.50              |
| 23:DB:2831:G:O4'   | 23:DB:2883:A:C2   | 2.65                     | 0.50              |
| 23:DB:2849:U:H4'   | 23:DB:2868:A:C2   | 2.46                     | 0.50              |
| 27:DE:163:ASN:N    | 27:DE:168:ASP:HA  | 2.25                     | 0.50              |
| 29:DG:23:ILE:O     | 29:DG:23:ILE:HG13 | 2.11                     | 0.50              |
| 29:DG:137:LYS:O    | 29:DG:140:ILE:HB  | 2.10                     | 0.50              |
| 31:DJ:125:TYR:OH   | 31:DJ:134:ALA:HB2 | 2.10                     | 0.50              |
| 38:DQ:60:TRP:CZ3   | 38:DQ:93:ILE:HG22 | 2.47                     | 0.50              |
| 45:DY:25:GLY:C     | 45:DY:26:LEU:HD23 | 2.36                     | 0.50              |
| 48:D1:24:LYS:HZ2   | 48:D1:25:ASN:N    | 2.10                     | 0.50              |
| 50:D3:56:LEU:C     | 50:D3:56:LEU:HD12 | 2.36                     | 0.50              |
| 1:AA:309:A:H2'     | 1:AA:310:G:H8     | 1.76                     | 0.50              |
| 1:AA:761:G:H2'     | 1:AA:762:U:C6     | 2.46                     | 0.50              |
| 1:AA:957:U:H4'     | 18:AS:78:THR:HB   | 1.93                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1252:A:H2'    | 1:AA:1253:G:C5'    | 2.39                     | 0.50              |
| 1:AA:1302:C:O4'    | 12:AM:16:ILE:HD11  | 2.12                     | 0.50              |
| 1:AA:1376:U:H2'    | 1:AA:1377:A:C8     | 2.45                     | 0.50              |
| 1:AA:1499:A:OP1    | 53:AA:1601:KSG:N1  | 2.45                     | 0.50              |
| 2:AC:55:VAL:HG12   | 2:AC:56:ILE:N      | 2.26                     | 0.50              |
| 2:AC:173:PRO:C     | 2:AC:175:HIS:H     | 2.19                     | 0.50              |
| 3:AD:120:LYS:HB2   | 3:AD:145:ARG:HH21  | 1.75                     | 0.50              |
| 12:AM:10:ASP:HA    | 12:AM:44:ILE:CD1   | 2.41                     | 0.50              |
| 17:AR:70:THR:HG23  | 17:AR:71:ASP:N     | 2.27                     | 0.50              |
| 19:AT:27:MET:HE1   | 19:AT:66:ILE:CG1   | 2.38                     | 0.50              |
| 20:AB:112:ARG:HA   | 20:AB:115:ASP:OD2  | 2.11                     | 0.50              |
| 23:BB:543:G:H2'    | 23:BB:544:C:C5'    | 2.35                     | 0.50              |
| 23:BB:550:C:H2'    | 23:BB:550:C:O2     | 2.10                     | 0.50              |
| 23:BB:771:G:O2'    | 23:BB:772:C:H5'    | 2.11                     | 0.50              |
| 23:BB:1159:U:O2'   | 23:BB:1160:G:H5'   | 2.11                     | 0.50              |
| 23:BB:1412:U:H2'   | 23:BB:1413:A:H8    | 1.76                     | 0.50              |
| 23:BB:1511:G:H2'   | 23:BB:1512:C:H6    | 1.77                     | 0.50              |
| 23:BB:1676:A:H1'   | 26:BD:134:HIS:HB3  | 1.94                     | 0.50              |
| 23:BB:2248:C:C2'   | 23:BB:2249:U:H5'   | 2.40                     | 0.50              |
| 23:BB:2370:G:H2'   | 23:BB:2371:G:O4'   | 2.10                     | 0.50              |
| 23:BB:2700:A:H2'   | 23:BB:2701:U:H6    | 1.76                     | 0.50              |
| 25:BC:266:ILE:O    | 25:BC:266:ILE:HG13 | 2.10                     | 0.50              |
| 26:BD:170:VAL:HG11 | 26:BD:194:PRO:HG2  | 1.92                     | 0.50              |
| 27:BE:44:ARG:CD    | 27:BE:44:ARG:N     | 2.73                     | 0.50              |
| 27:BE:144:GLU:C    | 27:BE:146:VAL:N    | 2.70                     | 0.50              |
| 29:BG:17:LYS:O     | 29:BG:17:LYS:HD2   | 2.09                     | 0.50              |
| 31:BJ:28:LEU:HG    | 31:BJ:32:LEU:CD1   | 2.41                     | 0.50              |
| 31:BJ:43:GLU:O     | 31:BJ:44:TYR:C     | 2.54                     | 0.50              |
| 31:BJ:101:ILE:HG23 | 31:BJ:102:GLU:N    | 2.20                     | 0.50              |
| 36:BO:94:ARG:O     | 36:BO:95:SER:C     | 2.54                     | 0.50              |
| 42:BU:21:ARG:HH11  | 42:BU:21:ARG:HG2   | 1.76                     | 0.50              |
| 52:BI:49:GLU:HG2   | 52:BI:54:ILE:HD11  | 1.93                     | 0.50              |
| 1:CA:114:U:H2'     | 1:CA:115:G:C8      | 2.47                     | 0.50              |
| 1:CA:638:U:H2'     | 1:CA:639:G:O4'     | 2.11                     | 0.50              |
| 1:CA:846:G:N3      | 1:CA:846:G:H2'     | 2.27                     | 0.50              |
| 1:CA:1254:A:H61    | 1:CA:1283:U:H3     | 1.60                     | 0.50              |
| 1:CA:1308:U:H2'    | 1:CA:1309:G:H8     | 1.75                     | 0.50              |
| 1:CA:1526:G:H2'    | 1:CA:1527:U:C6     | 2.46                     | 0.50              |
| 2:CC:61:LYS:HZ3    | 2:CC:96:VAL:CG1    | 2.25                     | 0.50              |
| 2:CC:69:THR:HG21   | 2:CC:75:VAL:HG21   | 1.94                     | 0.50              |
| 4:CE:152:VAL:HA    | 4:CE:155:LYS:HD3   | 1.93                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:CF:42:TRP:H     | 5:CF:42:TRP:CD1    | 2.30                     | 0.50              |
| 10:CK:23:HIS:HB3  | 10:CK:30:ILE:CG1   | 2.39                     | 0.50              |
| 12:CM:55:LEU:O    | 12:CM:59:VAL:HG12  | 2.11                     | 0.50              |
| 13:CN:9:GLU:OE2   | 13:CN:60:ARG:HB3   | 2.12                     | 0.50              |
| 15:CP:36:VAL:HG23 | 15:CP:56:ARG:HB2   | 1.93                     | 0.50              |
| 19:CT:24:ARG:HA   | 19:CT:65:LEU:HD21  | 1.94                     | 0.50              |
| 23:DB:145:C:H2'   | 23:DB:146:A:H8     | 1.77                     | 0.50              |
| 23:DB:279:A:H2'   | 23:DB:280:U:O4'    | 2.11                     | 0.50              |
| 23:DB:439:A:O2'   | 23:DB:440:C:H5'    | 2.11                     | 0.50              |
| 23:DB:490:C:H3'   | 23:DB:491:G:C5'    | 2.42                     | 0.50              |
| 23:DB:674:G:O2'   | 27:DE:69:ARG:HD2   | 2.12                     | 0.50              |
| 23:DB:786:C:O2'   | 23:DB:787:C:H5'    | 2.10                     | 0.50              |
| 23:DB:1562:U:H2'  | 23:DB:1563:U:C6    | 2.46                     | 0.50              |
| 23:DB:2665:A:C2'  | 23:DB:2666:C:H5'   | 2.41                     | 0.50              |
| 23:DB:2886:A:N7   | 47:D0:27:LEU:HG    | 2.26                     | 0.50              |
| 25:DC:92:LEU:HD13 | 25:DC:102:TYR:CE2  | 2.47                     | 0.50              |
| 25:DC:243:PRO:HA  | 25:DC:249:VAL:HG23 | 1.93                     | 0.50              |
| 27:DE:10:SER:C    | 27:DE:12:LEU:H     | 2.19                     | 0.50              |
| 29:DG:102:ILE:O   | 29:DG:102:ILE:HG23 | 2.12                     | 0.50              |
| 30:DH:62:LEU:O    | 30:DH:66:ASN:HB2   | 2.12                     | 0.50              |
| 33:DL:55:MET:H    | 33:DL:56:PRO:CD    | 2.25                     | 0.50              |
| 35:DN:33:ILE:HG23 | 35:DN:112:TYR:HB3  | 1.93                     | 0.50              |
| 35:DN:54:LEU:HD22 | 35:DN:66:ALA:HB2   | 1.94                     | 0.50              |
| 38:DQ:63:ARG:HG3  | 38:DQ:96:ASP:OD1   | 2.12                     | 0.50              |
| 39:DR:85:LYS:O    | 39:DR:86:GLN:HB3   | 2.10                     | 0.50              |
| 40:DS:72:THR:HG21 | 40:DS:108:SER:OG   | 2.11                     | 0.50              |
| 41:DT:76:ARG:NH1  | 41:DT:78:SER:HB2   | 2.16                     | 0.50              |
| 43:DW:77:LYS:C    | 43:DW:79:ILE:N     | 2.68                     | 0.50              |
| 47:D0:26:SER:HB2  | 47:D0:38:LEU:CG    | 2.42                     | 0.50              |
| 52:DI:116:MET:HE1 | 52:DI:128:ILE:HG12 | 1.94                     | 0.50              |
| 1:AA:372:C:H4'    | 1:AA:373:A:H5'     | 1.94                     | 0.50              |
| 1:AA:602:A:O2'    | 1:AA:603:U:H5'     | 2.11                     | 0.50              |
| 1:AA:638:U:H2'    | 1:AA:639:G:O4'     | 2.11                     | 0.50              |
| 1:AA:697:U:H2'    | 1:AA:698:G:H5'     | 1.93                     | 0.50              |
| 1:AA:751:U:H2'    | 1:AA:752:G:O4'     | 2.12                     | 0.50              |
| 1:AA:751:U:H4'    | 14:AO:23:SER:HA    | 1.92                     | 0.50              |
| 1:AA:812:G:O2'    | 1:AA:813:U:C6      | 2.58                     | 0.50              |
| 1:AA:1507:A:H2'   | 1:AA:1508:A:C8     | 2.47                     | 0.50              |
| 2:AC:102:ILE:C    | 2:AC:102:ILE:HD12  | 2.36                     | 0.50              |
| 2:AC:126:ARG:HH22 | 2:AC:190:THR:CG2   | 2.25                     | 0.50              |
| 5:AF:99:ALA:O     | 5:AF:100:SER:HB2   | 2.11                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:AK:54:SER:HA    | 10:AK:56:LYS:HE3   | 1.92                     | 0.50              |
| 15:AP:42:ILE:CG2   | 15:AP:43:ALA:H     | 2.18                     | 0.50              |
| 20:AB:49:PHE:O     | 20:AB:53:LEU:HD23  | 2.11                     | 0.50              |
| 23:BB:103:A:H2'    | 23:BB:104:A:O4'    | 2.12                     | 0.50              |
| 23:BB:1019:U:OP1   | 23:BB:1035:U:O2'   | 2.29                     | 0.50              |
| 23:BB:1080:A:O2'   | 23:BB:1081:U:H5'   | 2.10                     | 0.50              |
| 23:BB:1818:U:C3'   | 25:BC:155:ARG:HB2  | 2.41                     | 0.50              |
| 23:BB:2052:A:O5'   | 26:BD:147:GLY:HA3  | 2.12                     | 0.50              |
| 23:BB:2143:C:H2'   | 23:BB:2144:G:O4'   | 2.10                     | 0.50              |
| 23:BB:2256:G:O2'   | 23:BB:2257:U:H5'   | 2.12                     | 0.50              |
| 23:BB:2516:A:O2'   | 23:BB:2517:C:H5'   | 2.12                     | 0.50              |
| 23:BB:2665:A:C2'   | 23:BB:2666:C:H5'   | 2.41                     | 0.50              |
| 23:BB:2740:A:H2'   | 23:BB:2741:A:C8    | 2.46                     | 0.50              |
| 24:BV:76:ASP:HB2   | 34:BM:136:MET:SD   | 2.52                     | 0.50              |
| 25:BC:155:ARG:HH11 | 25:BC:157:ALA:HB2  | 1.76                     | 0.50              |
| 26:BD:7:LYS:HE2    | 26:BD:193:VAL:HG13 | 1.92                     | 0.50              |
| 26:BD:29:VAL:HA    | 26:BD:185:ASN:CG   | 2.37                     | 0.50              |
| 26:BD:114:LYS:HB3  | 35:BN:3:HIS:CE1    | 2.46                     | 0.50              |
| 32:BK:99:ILE:HG22  | 32:BK:119:ALA:HB2  | 1.93                     | 0.50              |
| 35:BN:17:ARG:O     | 35:BN:21:PHE:HB2   | 2.11                     | 0.50              |
| 36:BO:54:VAL:HG21  | 36:BO:78:VAL:HG11  | 1.94                     | 0.50              |
| 39:BR:75:VAL:N     | 39:BR:90:ARG:HE    | 2.07                     | 0.50              |
| 47:B0:46:GLY:HA3   | 47:B0:53:VAL:HG21  | 1.94                     | 0.50              |
| 48:B1:31:GLU:H     | 48:B1:32:LYS:HZ1   | 1.59                     | 0.50              |
| 1:CA:370:C:H2'     | 1:CA:371:A:C8      | 2.46                     | 0.50              |
| 1:CA:761:G:H2'     | 1:CA:762:U:C6      | 2.46                     | 0.50              |
| 1:CA:963:G:H2'     | 1:CA:964:A:H8      | 1.75                     | 0.50              |
| 1:CA:973:G:H3'     | 1:CA:974:A:C5'     | 2.30                     | 0.50              |
| 6:CG:16:LYS:O      | 6:CG:16:LYS:HD3    | 2.11                     | 0.50              |
| 7:CH:17:GLN:HG3    | 7:CH:71:VAL:CG2    | 2.41                     | 0.50              |
| 13:CN:13:VAL:HG13  | 13:CN:59:GLN:HE22  | 1.76                     | 0.50              |
| 15:CP:32:PHE:C     | 15:CP:32:PHE:CD1   | 2.90                     | 0.50              |
| 18:CS:52:ASN:ND2   | 18:CS:76:THR:HA    | 2.26                     | 0.50              |
| 20:CB:206:ILE:HG22 | 20:CB:207:ARG:NH2  | 2.26                     | 0.50              |
| 22:DA:31:C:O2'     | 22:DA:53:A:N1      | 2.44                     | 0.50              |
| 23:DB:363:G:H2'    | 23:DB:364:C:H6     | 1.74                     | 0.50              |
| 23:DB:910:A:C8     | 34:DM:16:ARG:HB3   | 2.47                     | 0.50              |
| 23:DB:1396:U:O4'   | 23:DB:1396:U:O2    | 2.28                     | 0.50              |
| 23:DB:1681:G:H2'   | 23:DB:1757:A:N1    | 2.27                     | 0.50              |
| 23:DB:2056:G:H21   | 47:D0:1:ALA:HB3    | 1.76                     | 0.50              |
| 23:DB:2412:A:H2'   | 23:DB:2413:G:O4'   | 2.11                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DB:2636:C:H2'   | 23:DB:2637:U:C6   | 2.46                     | 0.50              |
| 23:DB:2636:C:P     | 26:DD:80:TRP:HE1  | 2.34                     | 0.50              |
| 23:DB:2743:U:C3'   | 23:DB:2744:G:H5'' | 2.42                     | 0.50              |
| 25:DC:3:VAL:HG12   | 25:DC:4:LYS:N     | 2.27                     | 0.50              |
| 25:DC:103:ILE:HG22 | 25:DC:104:LEU:H   | 1.77                     | 0.50              |
| 25:DC:207:ALA:HA   | 25:DC:211:ARG:HB3 | 1.94                     | 0.50              |
| 26:DD:60:VAL:O     | 26:DD:63:PRO:HD2  | 2.12                     | 0.50              |
| 26:DD:117:GLY:O    | 26:DD:164:GLN:HA  | 2.12                     | 0.50              |
| 27:DE:192:ALA:HB1  | 27:DE:199:MET:CG  | 2.42                     | 0.50              |
| 31:DJ:5:THR:HG21   | 31:DJ:7:LYS:NZ    | 2.26                     | 0.50              |
| 31:DJ:37:ARG:NH1   | 31:DJ:110:PRO:HG3 | 2.27                     | 0.50              |
| 33:DL:58:TYR:HA    | 33:DL:62:PRO:CD   | 2.42                     | 0.50              |
| 33:DL:118:THR:CG2  | 33:DL:137:ALA:HB3 | 2.41                     | 0.50              |
| 34:DM:127:LYS:NZ   | 34:DM:129:THR:H   | 2.08                     | 0.50              |
| 35:DN:115:LEU:HD23 | 35:DN:115:LEU:N   | 2.26                     | 0.50              |
| 36:DO:80:GLU:O     | 36:DO:83:LEU:HD13 | 2.10                     | 0.50              |
| 37:DP:100:ARG:H    | 37:DP:100:ARG:CD  | 2.25                     | 0.50              |
| 37:DP:111:GLU:C    | 37:DP:113:LEU:H   | 2.18                     | 0.50              |
| 38:DQ:5:ARG:O      | 38:DQ:5:ARG:HD2   | 2.11                     | 0.50              |
| 40:DS:42:LYS:O     | 40:DS:42:LYS:HD3  | 2.11                     | 0.50              |
| 40:DS:64:ALA:H     | 40:DS:110:ARG:NH2 | 2.10                     | 0.50              |
| 43:DW:48:ALA:O     | 43:DW:72:GLY:HA3  | 2.12                     | 0.50              |
| 52:DI:99:LYS:HD3   | 52:DI:99:LYS:N    | 2.26                     | 0.50              |
| 1:AA:60:A:H1'      | 1:AA:61:G:O4'     | 2.12                     | 0.50              |
| 1:AA:437:U:C2'     | 1:AA:438:U:O4'    | 2.51                     | 0.50              |
| 1:AA:769:G:O2'     | 1:AA:770:C:H5'    | 2.11                     | 0.50              |
| 1:AA:864:A:H2'     | 1:AA:865:A:C8     | 2.46                     | 0.50              |
| 1:AA:1004:A:H62    | 1:AA:1025:U:H5'   | 1.77                     | 0.50              |
| 1:AA:1210:C:O2'    | 1:AA:1211:U:H5'   | 2.11                     | 0.50              |
| 1:AA:1504:G:H4'    | 1:AA:1505:G:C4    | 2.47                     | 0.50              |
| 2:AC:71:ARG:O      | 2:AC:75:VAL:HG23  | 2.11                     | 0.50              |
| 2:AC:183:TYR:HE1   | 2:AC:198:LYS:HB3  | 1.75                     | 0.50              |
| 5:AF:45:ARG:HG2    | 5:AF:46:GLN:N     | 2.26                     | 0.50              |
| 6:AG:46:LEU:HD13   | 6:AG:46:LEU:O     | 2.11                     | 0.50              |
| 8:AI:11:ARG:O      | 8:AI:11:ARG:HG3   | 2.10                     | 0.50              |
| 23:BB:408:G:O2'    | 23:BB:409:G:H5'   | 2.12                     | 0.50              |
| 23:BB:557:C:H2'    | 23:BB:558:U:H6    | 1.76                     | 0.50              |
| 23:BB:833:A:H2'    | 23:BB:834:G:H8    | 1.74                     | 0.50              |
| 23:BB:1373:A:OP1   | 23:BB:2213:U:O4   | 2.29                     | 0.50              |
| 23:BB:1531:C:H2'   | 23:BB:1532:A:H8   | 1.75                     | 0.50              |
| 23:BB:1796:U:H2'   | 23:BB:1797:G:C8   | 2.46                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:BB:2025:C:H2'   | 23:BB:2026:U:H6   | 1.77                     | 0.50              |
| 23:BB:2262:U:H4'   | 23:BB:2328:A:H2   | 1.76                     | 0.50              |
| 23:BB:2334:U:OP2   | 36:BO:7:ARG:HA    | 2.11                     | 0.50              |
| 23:BB:2439:A:C8    | 23:BB:2586:U:H4'  | 2.47                     | 0.50              |
| 25:BC:61:TYR:CE2   | 25:BC:63:ILE:HD11 | 2.47                     | 0.50              |
| 25:BC:66:PHE:O     | 25:BC:67:LYS:C    | 2.55                     | 0.50              |
| 25:BC:161:VAL:H    | 25:BC:193:GLU:CD  | 2.20                     | 0.50              |
| 27:BE:131:THR:O    | 27:BE:134:LEU:HB2 | 2.12                     | 0.50              |
| 27:BE:139:LYS:HE2  | 27:BE:139:LYS:HA  | 1.93                     | 0.50              |
| 28:BF:168:LEU:HD12 | 28:BF:169:LEU:N   | 2.15                     | 0.50              |
| 29:BG:18:ILE:H     | 29:BG:18:ILE:CD1  | 2.25                     | 0.50              |
| 30:BH:1:MET:C      | 30:BH:21:VAL:HG12 | 2.37                     | 0.50              |
| 30:BH:58:LEU:HA    | 30:BH:62:LEU:HD12 | 1.94                     | 0.50              |
| 32:BK:23:LYS:HG3   | 32:BK:24:VAL:H    | 1.75                     | 0.50              |
| 33:BL:109:LYS:HA   | 33:BL:126:ARG:CB  | 2.42                     | 0.50              |
| 36:BO:31:THR:HG21  | 36:BO:36:TYR:CE1  | 2.46                     | 0.50              |
| 38:BQ:40:LYS:HA    | 38:BQ:43:GLN:HE21 | 1.77                     | 0.50              |
| 42:BU:82:VAL:HB    | 42:BU:94:PHE:CD2  | 2.47                     | 0.50              |
| 50:B3:7:ARG:HH21   | 50:B3:11:LYS:HZ2  | 1.57                     | 0.50              |
| 50:B3:24:LYS:HZ3   | 50:B3:29:ARG:HH22 | 1.58                     | 0.50              |
| 1:CA:143:A:H2      | 1:CA:220:G:H22    | 1.59                     | 0.50              |
| 1:CA:1008:U:H5''   | 13:CN:23:ARG:NH2  | 2.20                     | 0.50              |
| 1:CA:1118:U:H5'    | 1:CA:1118:U:H6    | 1.76                     | 0.50              |
| 1:CA:1200:C:H4'    | 1:CA:1201:A:H5'   | 1.94                     | 0.50              |
| 1:CA:1221:G:OP1    | 18:CS:35:ARG:HD2  | 2.11                     | 0.50              |
| 1:CA:1427:C:O2'    | 1:CA:1428:A:H5'   | 2.11                     | 0.50              |
| 1:CA:1492:A:N6     | 1:CA:1494:G:C8    | 2.80                     | 0.50              |
| 2:CC:61:LYS:HZ3    | 2:CC:61:LYS:HB3   | 1.77                     | 0.50              |
| 3:CD:169:TRP:CE3   | 3:CD:185:PRO:HB3  | 2.46                     | 0.50              |
| 4:CE:15:ILE:HG22   | 4:CE:16:ALA:H     | 1.77                     | 0.50              |
| 4:CE:52:ALA:HB2    | 4:CE:61:LYS:HE2   | 1.93                     | 0.50              |
| 4:CE:131:ASN:C     | 4:CE:135:VAL:HG23 | 2.35                     | 0.50              |
| 5:CF:29:ILE:HG21   | 5:CF:64:VAL:HG11  | 1.93                     | 0.50              |
| 9:CJ:66:GLU:HG2    | 9:CJ:67:ILE:H     | 1.77                     | 0.50              |
| 13:CN:40:ARG:O     | 13:CN:45:LEU:HD11 | 2.11                     | 0.50              |
| 13:CN:42:ASN:HA    | 13:CN:45:LEU:HD12 | 1.94                     | 0.50              |
| 15:CP:25:ARG:HD3   | 15:CP:25:ARG:H    | 1.76                     | 0.50              |
| 20:CB:115:ASP:O    | 20:CB:119:GLN:HG2 | 2.12                     | 0.50              |
| 22:DA:66:A:N6      | 22:DA:107:G:C5    | 2.79                     | 0.50              |
| 23:DB:46:G:H2'     | 23:DB:47:C:H6     | 1.77                     | 0.50              |
| 23:DB:935:C:H2'    | 23:DB:936:A:C8    | 2.47                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:969:G:OP1    | 45:DY:17:PRO:HG3   | 2.11                     | 0.50              |
| 23:DB:1205:A:C8    | 27:DE:165:HIS:HA   | 2.47                     | 0.50              |
| 23:DB:1313:U:H4'   | 23:DB:1332:G:H4'   | 1.94                     | 0.50              |
| 23:DB:2020:A:C2    | 23:DB:2022:U:O4'   | 2.64                     | 0.50              |
| 23:DB:2405:G:H1'   | 23:DB:2412:A:H61   | 1.75                     | 0.50              |
| 23:DB:2742:G:O2'   | 23:DB:2743:U:H5'   | 2.12                     | 0.50              |
| 23:DB:2771:C:H2'   | 23:DB:2772:C:H6    | 1.76                     | 0.50              |
| 25:DC:171:VAL:HG23 | 25:DC:182:LYS:HZ3  | 1.76                     | 0.50              |
| 25:DC:178:GLY:C    | 25:DC:179:GLU:HG2  | 2.35                     | 0.50              |
| 25:DC:216:ARG:O    | 25:DC:218:THR:N    | 2.44                     | 0.50              |
| 25:DC:268:ARG:HG3  | 25:DC:268:ARG:HH11 | 1.77                     | 0.50              |
| 26:DD:146:ILE:H    | 26:DD:146:ILE:CD1  | 2.24                     | 0.50              |
| 27:DE:142:ALA:N    | 27:DE:185:LYS:NZ   | 2.52                     | 0.50              |
| 28:DF:98:PHE:HA    | 28:DF:101:ARG:HG2  | 1.93                     | 0.50              |
| 30:DH:122:LEU:HD13 | 30:DH:146:VAL:CG2  | 2.36                     | 0.50              |
| 32:DK:11:ALA:O     | 32:DK:99:ILE:HG23  | 2.10                     | 0.50              |
| 35:DN:10:LEU:O     | 35:DN:11:ASN:ND2   | 2.45                     | 0.50              |
| 35:DN:73:ASN:HA    | 35:DN:76:VAL:HG12  | 1.93                     | 0.50              |
| 37:DP:25:VAL:O     | 37:DP:27:VAL:HG12  | 2.11                     | 0.50              |
| 39:DR:47:VAL:HG22  | 39:DR:48:LYS:N     | 2.18                     | 0.50              |
| 41:DT:53:VAL:HB    | 41:DT:93:LEU:HD21  | 1.93                     | 0.50              |
| 44:DX:16:THR:OG1   | 44:DX:19:LEU:HB3   | 2.12                     | 0.50              |
| 51:D4:22:VAL:HG13  | 51:D4:37:GLN:HB3   | 1.93                     | 0.50              |
| 1:AA:146:G:O2'     | 1:AA:147:G:H5'     | 2.11                     | 0.50              |
| 1:AA:251:G:H4'     | 1:AA:252:U:H5'     | 1.93                     | 0.50              |
| 1:AA:323:U:H2'     | 1:AA:324:G:O4'     | 2.11                     | 0.50              |
| 1:AA:980:C:H2'     | 1:AA:981:U:H5'     | 1.93                     | 0.50              |
| 1:AA:1261:A:H2'    | 1:AA:1262:C:O4'    | 2.11                     | 0.50              |
| 1:AA:1324:A:H2'    | 1:AA:1325:C:C6     | 2.47                     | 0.50              |
| 2:AC:155:ARG:NH1   | 2:AC:192:TYR:HB2   | 2.27                     | 0.50              |
| 4:AE:101:GLY:H     | 4:AE:121:ASN:ND2   | 2.07                     | 0.50              |
| 7:AH:76:ARG:HE     | 7:AH:79:ARG:HA     | 1.77                     | 0.50              |
| 8:AI:50:PRO:HG2    | 8:AI:51:LEU:HD12   | 1.92                     | 0.50              |
| 20:AB:80:LYS:O     | 20:AB:84:LEU:N     | 2.45                     | 0.50              |
| 20:AB:204:ASP:CG   | 20:AB:205:ALA:N    | 2.70                     | 0.50              |
| 22:BA:32:U:H4'     | 22:BA:52:A:H62     | 1.76                     | 0.50              |
| 23:BB:235:U:H2'    | 23:BB:236:C:H6     | 1.76                     | 0.50              |
| 23:BB:536:G:H4'    | 38:BQ:56:PHE:HZ    | 1.74                     | 0.50              |
| 23:BB:855:G:N2     | 43:BW:23:LYS:HB3   | 2.26                     | 0.50              |
| 23:BB:988:A:OP2    | 45:BY:11:SER:HA    | 2.12                     | 0.50              |
| 23:BB:993:G:O2'    | 23:BB:994:C:H5'    | 2.11                     | 0.50              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:1236:G:O2'  | 23:BB:1237:A:O5'   | 2.29                     | 0.50              |
| 23:BB:1313:U:H4'  | 23:BB:1332:G:H4'   | 1.94                     | 0.50              |
| 23:BB:1396:U:O2   | 23:BB:1396:U:O4'   | 2.28                     | 0.50              |
| 23:BB:1909:C:H2'  | 23:BB:1910:G:H8    | 1.77                     | 0.50              |
| 23:BB:2020:A:C2   | 23:BB:2022:U:O4'   | 2.64                     | 0.50              |
| 23:BB:2485:G:H5'  | 34:BM:45:GLN:OE1   | 2.12                     | 0.50              |
| 23:BB:2669:G:H2'  | 23:BB:2670:A:H8    | 1.76                     | 0.50              |
| 23:BB:2675:A:OP1  | 32:BK:31:ARG:HG2   | 2.10                     | 0.50              |
| 23:BB:2821:A:H2'  | 23:BB:2822:G:C8    | 2.46                     | 0.50              |
| 23:BB:2822:G:OP1  | 26:BD:166:GLY:HA2  | 2.11                     | 0.50              |
| 25:BC:67:LYS:HB3  | 25:BC:149:LYS:O    | 2.12                     | 0.50              |
| 25:BC:77:VAL:HA   | 25:BC:93:VAL:HG22  | 1.94                     | 0.50              |
| 25:BC:136:VAL:O   | 25:BC:163:ILE:HB   | 2.12                     | 0.50              |
| 25:BC:198:GLU:C   | 25:BC:200:MET:H    | 2.18                     | 0.50              |
| 27:BE:57:LYS:O    | 27:BE:59:PRO:HD3   | 2.11                     | 0.50              |
| 27:BE:104:ALA:O   | 27:BE:105:LEU:HD23 | 2.12                     | 0.50              |
| 27:BE:170:ARG:NH2 | 27:BE:175:ILE:HA   | 2.26                     | 0.50              |
| 28:BF:106:ALA:CB  | 28:BF:136:ILE:HG23 | 2.42                     | 0.50              |
| 30:BH:85:GLY:O    | 30:BH:89:LYS:N     | 2.45                     | 0.50              |
| 31:BJ:59:ALA:C    | 31:BJ:61:LYS:H     | 2.20                     | 0.50              |
| 32:BK:7:MET:HE2   | 32:BK:7:MET:HA     | 1.93                     | 0.50              |
| 32:BK:10:VAL:HG13 | 32:BK:19:VAL:HG21  | 1.94                     | 0.50              |
| 33:BL:92:LEU:HG   | 33:BL:96:LYS:NZ    | 2.27                     | 0.50              |
| 34:BM:26:VAL:HG11 | 34:BM:134:THR:OG1  | 2.12                     | 0.50              |
| 36:BO:59:ALA:HB3  | 36:BO:63:LYS:HB2   | 1.93                     | 0.50              |
| 37:BP:61:ARG:O    | 37:BP:63:ILE:HD12  | 2.11                     | 0.50              |
| 38:BQ:7:VAL:HG23  | 38:BQ:8:ILE:N      | 2.18                     | 0.50              |
| 38:BQ:13:HIS:O    | 38:BQ:17:LEU:HB2   | 2.12                     | 0.50              |
| 38:BQ:88:GLU:HA   | 39:BR:53:PHE:CD1   | 2.47                     | 0.50              |
| 38:BQ:111:LYS:O   | 38:BQ:115:ALA:HB2  | 2.12                     | 0.50              |
| 47:B0:11:LYS:O    | 47:B0:12:ARG:HB3   | 2.12                     | 0.50              |
| 48:B1:36:LYS:HD2  | 48:B1:36:LYS:N     | 2.27                     | 0.50              |
| 1:CA:806:C:H2'    | 1:CA:807:A:C8      | 2.46                     | 0.50              |
| 1:CA:1026:G:H2'   | 1:CA:1027:C:O4'    | 2.12                     | 0.50              |
| 1:CA:1171:A:H2'   | 1:CA:1172:C:H6     | 1.77                     | 0.50              |
| 1:CA:1219:A:H2'   | 1:CA:1220:G:H8     | 1.75                     | 0.50              |
| 1:CA:1496:C:H2'   | 1:CA:1497:G:O4'    | 2.11                     | 0.50              |
| 1:CA:1512:U:H2'   | 1:CA:1513:A:H8     | 1.75                     | 0.50              |
| 3:CD:84:ASN:HD21  | 3:CD:87:GLU:H      | 1.58                     | 0.50              |
| 5:CF:68:GLN:O     | 5:CF:71:ILE:HG22   | 2.11                     | 0.50              |
| 6:CG:29:LEU:HD11  | 6:CG:119:LEU:HD22  | 1.94                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:CH:77:VAL:CG2   | 7:CH:126:CYS:HA    | 2.42                     | 0.50              |
| 12:CM:102:LYS:HG3 | 12:CM:103:THR:N    | 2.26                     | 0.50              |
| 23:DB:125:A:O2'   | 23:DB:126:A:OP1    | 2.24                     | 0.50              |
| 23:DB:242:G:H22   | 23:DB:254:G:H2'    | 1.76                     | 0.50              |
| 23:DB:299:A:H2'   | 23:DB:300:A:C8     | 2.46                     | 0.50              |
| 23:DB:441:U:H2'   | 23:DB:442:G:H8     | 1.76                     | 0.50              |
| 23:DB:725:G:H2'   | 23:DB:726:G:C1'    | 2.41                     | 0.50              |
| 23:DB:943:A:OP1   | 33:DL:41:ARG:HG2   | 2.12                     | 0.50              |
| 23:DB:1139:G:O2'  | 23:DB:1140:C:H5'   | 2.12                     | 0.50              |
| 23:DB:1948:G:O2'  | 23:DB:1949:G:H5'   | 2.12                     | 0.50              |
| 23:DB:2399:G:H1'  | 48:D1:20:TYR:OH    | 2.12                     | 0.50              |
| 23:DB:2420:C:H3'  | 50:D3:31:ILE:CG2   | 2.42                     | 0.50              |
| 23:DB:2464:G:H2'  | 23:DB:2465:C:H6    | 1.75                     | 0.50              |
| 23:DB:2500:U:H5'  | 23:DB:2501:C:OP2   | 2.12                     | 0.50              |
| 24:DV:57:TYR:HE2  | 24:DV:77:VAL:HG21  | 1.76                     | 0.50              |
| 27:DE:29:HIS:HD2  | 33:DL:19:LEU:HD11  | 1.76                     | 0.50              |
| 27:DE:199:MET:O   | 27:DE:200:LEU:HD23 | 2.12                     | 0.50              |
| 28:DF:174:PHE:N   | 28:DF:175:PRO:HD2  | 2.23                     | 0.50              |
| 34:DM:16:ARG:HG2  | 34:DM:16:ARG:HH11  | 1.77                     | 0.50              |
| 40:DS:22:ASP:C    | 40:DS:24:ILE:H     | 2.20                     | 0.50              |
| 41:DT:11:LEU:HB3  | 41:DT:34:VAL:HG23  | 1.92                     | 0.50              |
| 43:DW:42:THR:H    | 43:DW:65:LYS:CG    | 2.22                     | 0.50              |
| 48:D1:7:LYS:HZ3   | 48:D1:26:LYS:H     | 1.60                     | 0.50              |
| 51:D4:15:LYS:C    | 51:D4:17:VAL:H     | 2.20                     | 0.50              |
| 52:DI:21:PRO:CB   | 52:DI:22:PRO:HD3   | 2.39                     | 0.50              |
| 52:DI:85:ILE:HD12 | 52:DI:87:SER:O     | 2.12                     | 0.50              |
| 1:AA:130:A:O4'    | 16:AQ:64:ARG:HD2   | 2.12                     | 0.50              |
| 1:AA:143:A:H2     | 1:AA:220:G:H22     | 1.59                     | 0.50              |
| 1:AA:219:U:H2'    | 1:AA:220:G:H8      | 1.77                     | 0.50              |
| 1:AA:370:C:H2'    | 1:AA:371:A:H8      | 1.77                     | 0.50              |
| 1:AA:734:G:N2     | 17:AR:63:TYR:CE2   | 2.80                     | 0.50              |
| 1:AA:969:A:N3     | 1:AA:970:C:O2      | 2.45                     | 0.50              |
| 1:AA:1226:C:H4'   | 1:AA:1227:A:OP1    | 2.11                     | 0.50              |
| 3:AD:11:SER:OG    | 3:AD:17:ASP:HA     | 2.11                     | 0.50              |
| 3:AD:77:GLU:O     | 3:AD:81:LEU:HG     | 2.12                     | 0.50              |
| 5:AF:51:ILE:HD11  | 5:AF:86:ARG:HG3    | 1.94                     | 0.50              |
| 8:AI:49:GLN:N     | 8:AI:50:PRO:HD2    | 2.27                     | 0.50              |
| 22:BA:52:A:H3'    | 22:BA:53:A:C8      | 2.47                     | 0.50              |
| 23:BB:535:G:N2    | 38:BQ:52:ARG:HH22  | 1.95                     | 0.50              |
| 23:BB:827:U:H5'   | 23:BB:828:U:O5'    | 2.12                     | 0.50              |
| 23:BB:922:C:H2'   | 23:BB:923:G:C8     | 2.47                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:968:C:H2'    | 23:BB:969:G:C8     | 2.45                     | 0.50              |
| 23:BB:1386:C:H2'   | 23:BB:1387:A:H8    | 1.74                     | 0.50              |
| 23:BB:2809:A:H2'   | 23:BB:2810:A:H8    | 1.77                     | 0.50              |
| 25:BC:22:GLU:HA    | 25:BC:202:ARG:NE   | 2.26                     | 0.50              |
| 25:BC:130:PRO:HA   | 25:BC:187:CYS:O    | 2.12                     | 0.50              |
| 26:BD:45:TYR:O     | 26:BD:46:ARG:HG2   | 2.12                     | 0.50              |
| 26:BD:48:ILE:HA    | 26:BD:79:LEU:O     | 2.10                     | 0.50              |
| 27:BE:88:ARG:HH11  | 27:BE:88:ARG:CB    | 2.22                     | 0.50              |
| 27:BE:120:VAL:HG12 | 27:BE:121:VAL:N    | 2.27                     | 0.50              |
| 29:BG:102:ILE:HG22 | 29:BG:114:HIS:O    | 2.12                     | 0.50              |
| 30:BH:69:ALA:HB1   | 30:BH:141:LYS:NZ   | 2.27                     | 0.50              |
| 31:BJ:7:LYS:CD     | 31:BJ:48:VAL:HB    | 2.39                     | 0.50              |
| 31:BJ:61:LYS:HA    | 31:BJ:61:LYS:CE    | 2.38                     | 0.50              |
| 32:BK:16:ALA:N     | 32:BK:46:ALA:HA    | 2.27                     | 0.50              |
| 33:BL:116:VAL:HG21 | 33:BL:134:ALA:HB1  | 1.94                     | 0.50              |
| 35:BN:1:MET:SD     | 35:BN:2:ARG:N      | 2.85                     | 0.50              |
| 37:BP:61:ARG:NH2   | 37:BP:63:ILE:HD11  | 2.27                     | 0.50              |
| 38:BQ:56:PHE:O     | 38:BQ:59:LEU:HB3   | 2.12                     | 0.50              |
| 38:BQ:94:LEU:HD11  | 39:BR:10:LYS:HD2   | 1.94                     | 0.50              |
| 39:BR:49:ILE:HG22  | 39:BR:51:VAL:CG2   | 2.42                     | 0.50              |
| 40:BS:34:ASP:HA    | 40:BS:38:TYR:CD2   | 2.47                     | 0.50              |
| 41:BT:28:ASN:N     | 41:BT:28:ASN:HD22  | 2.09                     | 0.50              |
| 45:BY:6:ILE:HG22   | 45:BY:56:VAL:CG2   | 2.39                     | 0.50              |
| 45:BY:9:THR:HA     | 45:BY:55:LYS:HG3   | 1.92                     | 0.50              |
| 1:CA:1307:U:H2'    | 1:CA:1308:U:H6     | 1.76                     | 0.50              |
| 4:CE:59:ILE:HG22   | 4:CE:63:MET:HE2    | 1.94                     | 0.50              |
| 4:CE:111:ARG:HG2   | 4:CE:111:ARG:NH1   | 2.27                     | 0.50              |
| 5:CF:100:SER:H     | 17:CR:23:LYS:HZ1   | 1.60                     | 0.50              |
| 9:CJ:85:ASP:HB2    | 9:CJ:89:ARG:CZ     | 2.42                     | 0.50              |
| 10:CK:108:ASN:OD1  | 10:CK:110:THR:HG23 | 2.12                     | 0.50              |
| 11:CL:113:ARG:CZ   | 11:CL:120:ARG:HA   | 2.42                     | 0.50              |
| 13:CN:40:ARG:HH12  | 18:CS:6:LYS:H      | 1.59                     | 0.50              |
| 15:CP:74:LEU:O     | 15:CP:78:VAL:HG12  | 2.11                     | 0.50              |
| 18:CS:20:LYS:O     | 18:CS:20:LYS:HD2   | 2.12                     | 0.50              |
| 22:DA:30:C:C2'     | 22:DA:31:C:H5'     | 2.39                     | 0.50              |
| 23:DB:678:C:H2'    | 23:DB:679:C:H6     | 1.77                     | 0.50              |
| 23:DB:699:A:H4'    | 23:DB:1634:A:N7    | 2.27                     | 0.50              |
| 23:DB:1184:U:O2'   | 23:DB:1185:G:H5'   | 2.12                     | 0.50              |
| 23:DB:1330:C:H2'   | 23:DB:1331:G:H8    | 1.76                     | 0.50              |
| 23:DB:1771:C:H2'   | 23:DB:1772:A:C8    | 2.46                     | 0.50              |
| 23:DB:2052:A:OP1   | 26:DD:145:SER:HB3  | 2.12                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:2520:C:C6    | 23:DB:2567:G:H1'   | 2.46                     | 0.50              |
| 23:DB:2630:G:H2'   | 23:DB:2631:G:H8    | 1.75                     | 0.50              |
| 25:DC:192:GLY:O    | 25:DC:194:VAL:HG22 | 2.11                     | 0.50              |
| 26:DD:116:LYS:O    | 35:DN:2:ARG:HB3    | 2.12                     | 0.50              |
| 26:DD:160:LYS:HE3  | 26:DD:160:LYS:HA   | 1.93                     | 0.50              |
| 28:DF:137:PHE:O    | 28:DF:139:GLU:HG2  | 2.12                     | 0.50              |
| 33:DL:51:GLU:CG    | 33:DL:52:GLY:H     | 2.09                     | 0.50              |
| 34:DM:34:LYS:O     | 34:DM:125:PRO:HD2  | 2.12                     | 0.50              |
| 36:DO:95:SER:O     | 36:DO:97:PHE:N     | 2.45                     | 0.50              |
| 42:DU:48:VAL:C     | 42:DU:50:ALA:N     | 2.65                     | 0.50              |
| 52:DI:78:LEU:HD23  | 52:DI:81:LYS:HE2   | 1.93                     | 0.50              |
| 1:AA:193:C:H2'     | 1:AA:194:C:C6      | 2.47                     | 0.50              |
| 1:AA:939:G:H4'     | 6:AG:101:ARG:NH2   | 2.26                     | 0.50              |
| 1:AA:1446:A:C3'    | 1:AA:1447:A:H5''   | 2.42                     | 0.50              |
| 5:AF:100:SER:HA    | 17:AR:23:LYS:HZ2   | 1.77                     | 0.50              |
| 6:AG:72:VAL:HB     | 6:AG:144:ALA:HB3   | 1.94                     | 0.50              |
| 6:AG:136:LYS:O     | 6:AG:140:VAL:HG23  | 2.12                     | 0.50              |
| 8:AI:56:MET:CE     | 8:AI:57:VAL:H      | 2.25                     | 0.50              |
| 9:AJ:87:LEU:C      | 9:AJ:87:LEU:HD13   | 2.37                     | 0.50              |
| 14:AO:70:LYS:NZ    | 14:AO:74:VAL:HA    | 2.27                     | 0.50              |
| 15:AP:67:ILE:HG13  | 15:AP:71:VAL:HG13  | 1.93                     | 0.50              |
| 16:AQ:74:LEU:C     | 16:AQ:74:LEU:HD13  | 2.37                     | 0.50              |
| 19:AT:15:LYS:HA    | 19:AT:18:LYS:HE3   | 1.94                     | 0.50              |
| 21:AU:5:VAL:HG22   | 21:AU:19:LYS:NZ    | 2.27                     | 0.50              |
| 23:BB:189:G:P      | 46:BZ:12:ILE:HG12  | 2.52                     | 0.50              |
| 23:BB:1107:G:H2'   | 23:BB:1108:U:O4'   | 2.11                     | 0.50              |
| 23:BB:1399:C:H2'   | 23:BB:1400:U:C6    | 2.47                     | 0.50              |
| 23:BB:2087:G:H2'   | 23:BB:2088:A:H8    | 1.77                     | 0.50              |
| 23:BB:2305:U:H3    | 28:BF:150:GLY:HA3  | 1.76                     | 0.50              |
| 23:BB:2811:G:H5''  | 26:BD:62:LYS:HD2   | 1.93                     | 0.50              |
| 23:BB:2877:G:H2'   | 23:BB:2878:U:C6    | 2.47                     | 0.50              |
| 24:BV:80:HIS:CD2   | 24:BV:82:TYR:H     | 2.25                     | 0.50              |
| 27:BE:4:VAL:HB     | 27:BE:117:ARG:HH21 | 1.76                     | 0.50              |
| 27:BE:50:ALA:O     | 27:BE:74:LYS:HD2   | 2.12                     | 0.50              |
| 30:BH:6:LEU:HD12   | 30:BH:15:LEU:CA    | 2.42                     | 0.50              |
| 30:BH:56:ALA:HB3   | 30:BH:57:LYS:NZ    | 2.27                     | 0.50              |
| 30:BH:57:LYS:HE3   | 30:BH:57:LYS:CA    | 2.42                     | 0.50              |
| 31:BJ:18:VAL:HG22  | 31:BJ:56:VAL:HA    | 1.93                     | 0.50              |
| 31:BJ:36:LEU:O     | 31:BJ:118:MET:HG2  | 2.12                     | 0.50              |
| 34:BM:97:GLN:N     | 34:BM:98:PRO:CD    | 2.75                     | 0.50              |
| 34:BM:112:LEU:HD12 | 34:BM:112:LEU:N    | 2.27                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 36:BO:17:LYS:O     | 36:BO:21:LEU:HA   | 2.12                     | 0.50              |
| 40:BS:17:VAL:HA    | 40:BS:43:ALA:CB   | 2.42                     | 0.50              |
| 40:BS:57:ASN:O     | 40:BS:61:ASN:HB3  | 2.12                     | 0.50              |
| 41:BT:13:ALA:HB3   | 41:BT:33:LYS:HB2  | 1.92                     | 0.50              |
| 44:BX:5:GLU:N      | 44:BX:7:ARG:HE    | 2.08                     | 0.50              |
| 45:BY:27:GLY:C     | 45:BY:28:LEU:HD12 | 2.37                     | 0.50              |
| 46:BZ:49:ARG:CD    | 46:BZ:50:ASP:N    | 2.75                     | 0.50              |
| 1:CA:262:A:OP2     | 19:CT:70:LYS:HE3  | 2.12                     | 0.50              |
| 1:CA:372:C:H4'     | 1:CA:373:A:H5'    | 1.94                     | 0.50              |
| 1:CA:736:C:H2'     | 1:CA:737:C:H6     | 1.77                     | 0.50              |
| 1:CA:945:G:H21     | 1:CA:1334:G:H4'   | 1.77                     | 0.50              |
| 1:CA:1129:C:H1'    | 1:CA:1146:A:N6    | 2.25                     | 0.50              |
| 1:CA:1151:A:HO2'   | 1:CA:1152:A:H8    | 1.60                     | 0.50              |
| 4:CE:89:THR:C      | 4:CE:91:SER:N     | 2.69                     | 0.50              |
| 15:CP:67:ILE:CG1   | 15:CP:71:VAL:HG13 | 2.37                     | 0.50              |
| 16:CQ:13:SER:HB3   | 16:CQ:21:VAL:CB   | 2.40                     | 0.50              |
| 18:CS:11:ASP:HB3   | 18:CS:13:HIS:NE2  | 2.27                     | 0.50              |
| 18:CS:16:LYS:O     | 18:CS:20:LYS:HB2  | 2.11                     | 0.50              |
| 20:CB:134:LEU:HD23 | 20:CB:134:LEU:O   | 2.11                     | 0.50              |
| 21:CU:3:ILE:HD12   | 21:CU:3:ILE:O     | 2.11                     | 0.50              |
| 23:DB:19:A:OP1     | 38:DQ:22:GLY:HA2  | 2.12                     | 0.50              |
| 23:DB:217:A:H3'    | 23:DB:218:A:H8    | 1.75                     | 0.50              |
| 23:DB:416:U:H2'    | 23:DB:417:C:C6    | 2.46                     | 0.50              |
| 23:DB:553:G:O2'    | 23:DB:554:U:H5'   | 2.11                     | 0.50              |
| 23:DB:1196:C:H2'   | 23:DB:1197:G:C8   | 2.46                     | 0.50              |
| 23:DB:2191:A:H2'   | 23:DB:2192:U:C6   | 2.47                     | 0.50              |
| 23:DB:2682:A:O2'   | 23:DB:2683:C:H5'  | 2.11                     | 0.50              |
| 23:DB:2877:G:H2'   | 23:DB:2878:U:C6   | 2.47                     | 0.50              |
| 27:DE:28:VAL:O     | 27:DE:32:VAL:HG23 | 2.12                     | 0.50              |
| 27:DE:132:LYS:HG2  | 27:DE:134:LEU:CD1 | 2.41                     | 0.50              |
| 27:DE:164:LEU:HD13 | 27:DE:165:HIS:N   | 2.27                     | 0.50              |
| 29:DG:51:PHE:CE1   | 29:DG:53:PRO:HG3  | 2.45                     | 0.50              |
| 30:DH:114:GLU:CB   | 30:DH:133:GLN:HG3 | 2.37                     | 0.50              |
| 30:DH:116:ARG:HG2  | 30:DH:116:ARG:O   | 2.12                     | 0.50              |
| 31:DJ:76:HIS:HB2   | 31:DJ:86:GLN:CG   | 2.41                     | 0.50              |
| 31:DJ:78:THR:H     | 31:DJ:84:ILE:CD1  | 2.25                     | 0.50              |
| 33:DL:35:HIS:O     | 33:DL:35:HIS:CG   | 2.65                     | 0.50              |
| 33:DL:44:GLY:HA2   | 33:DL:47:ARG:NE   | 2.22                     | 0.50              |
| 36:DO:40:ILE:HD13  | 36:DO:40:ILE:N    | 2.16                     | 0.50              |
| 39:DR:72:VAL:O     | 39:DR:72:VAL:HG13 | 2.11                     | 0.50              |
| 41:DT:76:ARG:CG    | 41:DT:77:ARG:N    | 2.70                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:DX:18:LEU:HD12  | 44:DX:47:ARG:HH22  | 1.77                     | 0.50              |
| 51:D4:2:LYS:HD3    | 51:D4:2:LYS:N      | 2.27                     | 0.50              |
| 1:AA:33:A:H2'      | 1:AA:34:C:H6       | 1.77                     | 0.49              |
| 1:AA:968:A:O2'     | 1:AA:969:A:OP1     | 2.27                     | 0.49              |
| 1:AA:1169:A:H2'    | 1:AA:1170:A:C8     | 2.48                     | 0.49              |
| 1:AA:1332:A:H2'    | 1:AA:1333:A:C8     | 2.47                     | 0.49              |
| 1:AA:1458:G:H2'    | 1:AA:1459:G:H8     | 1.77                     | 0.49              |
| 3:AD:186:GLU:C     | 3:AD:190:LEU:HD13  | 2.37                     | 0.49              |
| 7:AH:29:SER:CB     | 7:AH:32:LYS:HZ2    | 2.25                     | 0.49              |
| 11:AL:20:VAL:O     | 11:AL:20:VAL:HG12  | 2.12                     | 0.49              |
| 16:AQ:10:ARG:NH2   | 16:AQ:58:VAL:HG13  | 2.27                     | 0.49              |
| 16:AQ:66:LEU:HD11  | 16:AQ:73:THR:CG2   | 2.41                     | 0.49              |
| 17:AR:44:THR:HG22  | 17:AR:46:THR:HB    | 1.95                     | 0.49              |
| 20:AB:46:VAL:O     | 20:AB:49:PHE:HB2   | 2.12                     | 0.49              |
| 20:AB:59:ILE:HD12  | 20:AB:59:ILE:C     | 2.37                     | 0.49              |
| 21:AU:26:GLY:O     | 21:AU:30:GLU:HB2   | 2.12                     | 0.49              |
| 23:BB:272:A:H2'    | 23:BB:273:G:C8     | 2.47                     | 0.49              |
| 23:BB:395:U:H2'    | 23:BB:396:G:C8     | 2.47                     | 0.49              |
| 23:BB:708:G:H2'    | 23:BB:709:U:C6     | 2.47                     | 0.49              |
| 23:BB:932:U:H2'    | 23:BB:934:U:C4     | 2.46                     | 0.49              |
| 23:BB:1054:A:H2'   | 23:BB:1055:G:C8    | 2.45                     | 0.49              |
| 23:BB:2526:G:H2'   | 23:BB:2527:C:C6    | 2.47                     | 0.49              |
| 25:BC:172:THR:HG22 | 25:BC:173:LEU:N    | 2.24                     | 0.49              |
| 25:BC:182:LYS:HE2  | 25:BC:264:LYS:NZ   | 2.27                     | 0.49              |
| 25:BC:222:THR:HG23 | 25:BC:231:HIS:CD2  | 2.47                     | 0.49              |
| 26:BD:8:LYS:HB3    | 37:BP:5:LYS:HZ2    | 1.74                     | 0.49              |
| 26:BD:18:ASP:O     | 32:BK:73:ASP:HA    | 2.11                     | 0.49              |
| 27:BE:191:ASP:C    | 27:BE:193:VAL:H    | 2.20                     | 0.49              |
| 29:BG:126:THR:HG23 | 29:BG:128:THR:HG23 | 1.93                     | 0.49              |
| 30:BH:5:LEU:HD21   | 30:BH:17:ASP:OD1   | 2.12                     | 0.49              |
| 32:BK:23:LYS:O     | 32:BK:39:ILE:HG23  | 2.12                     | 0.49              |
| 33:BL:18:ARG:HD3   | 33:BL:18:ARG:N     | 2.27                     | 0.49              |
| 34:BM:38:ARG:HA    | 34:BM:96:ILE:O     | 2.11                     | 0.49              |
| 37:BP:38:ARG:NH1   | 37:BP:39:LEU:N     | 2.59                     | 0.49              |
| 38:BQ:90:ASP:HA    | 39:BR:10:LYS:HZ3   | 1.76                     | 0.49              |
| 38:BQ:97:ILE:HD13  | 38:BQ:100:PHE:CZ   | 2.46                     | 0.49              |
| 42:BU:15:GLY:HA2   | 42:BU:18:LYS:HD3   | 1.92                     | 0.49              |
| 47:B0:46:GLY:O     | 47:B0:52:LYS:HB3   | 2.12                     | 0.49              |
| 1:CA:22:G:H2'      | 1:CA:23:C:C6       | 2.47                     | 0.49              |
| 1:CA:309:A:H2'     | 1:CA:310:G:H8      | 1.76                     | 0.49              |
| 1:CA:429:U:P       | 3:CD:12:ARG:HH21   | 2.35                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:751:U:H2'     | 1:CA:752:G:O4'     | 2.12                     | 0.49              |
| 1:CA:829:G:H4'     | 20:CB:24:PRO:HG3   | 1.94                     | 0.49              |
| 1:CA:1070:U:H2'    | 1:CA:1071:C:C6     | 2.47                     | 0.49              |
| 1:CA:1241:G:H2'    | 1:CA:1242:G:C8     | 2.42                     | 0.49              |
| 1:CA:1298:U:H2'    | 6:CG:113:LYS:NZ    | 2.27                     | 0.49              |
| 1:CA:1492:A:H2'    | 1:CA:1492:A:N3     | 2.26                     | 0.49              |
| 2:CC:61:LYS:NZ     | 2:CC:96:VAL:HG12   | 2.26                     | 0.49              |
| 2:CC:149:LYS:HE3   | 2:CC:200:TRP:CE3   | 2.47                     | 0.49              |
| 6:CG:55:LYS:HB3    | 6:CG:59:GLU:OE2    | 2.12                     | 0.49              |
| 10:CK:22:ILE:HG21  | 10:CK:95:THR:HG21  | 1.93                     | 0.49              |
| 10:CK:85:VAL:HG11  | 10:CK:96:ILE:HD11  | 1.93                     | 0.49              |
| 14:CO:72:LYS:O     | 14:CO:73:ASP:HB2   | 2.11                     | 0.49              |
| 18:CS:10:ILE:HD13  | 18:CS:40:PHE:CE2   | 2.47                     | 0.49              |
| 20:CB:45:THR:HG23  | 20:CB:200:PRO:HG2  | 1.94                     | 0.49              |
| 20:CB:212:TYR:O    | 20:CB:216:VAL:HG22 | 2.11                     | 0.49              |
| 22:DA:113:C:HO2'   | 36:DO:47:VAL:HA    | 1.76                     | 0.49              |
| 23:DB:351:C:H2'    | 23:DB:352:A:C8     | 2.46                     | 0.49              |
| 23:DB:1080:A:H4'   | 52:DI:126:ARG:HD3  | 1.93                     | 0.49              |
| 23:DB:1399:C:H2'   | 23:DB:1400:U:C6    | 2.47                     | 0.49              |
| 23:DB:1439:A:N7    | 23:DB:1440:U:C2    | 2.80                     | 0.49              |
| 23:DB:1501:G:O2'   | 23:DB:1502:A:H5'   | 2.11                     | 0.49              |
| 23:DB:1533:C:C2'   | 23:DB:1534:U:H5'   | 2.42                     | 0.49              |
| 23:DB:1796:U:H2'   | 23:DB:1797:G:C8    | 2.46                     | 0.49              |
| 23:DB:1813:G:C1'   | 25:DC:45:ASN:HB3   | 2.41                     | 0.49              |
| 23:DB:2106:U:H2'   | 23:DB:2107:G:OP1   | 2.12                     | 0.49              |
| 23:DB:2439:A:C8    | 23:DB:2586:U:H4'   | 2.47                     | 0.49              |
| 23:DB:2514:U:H2'   | 23:DB:2515:C:H6    | 1.77                     | 0.49              |
| 26:DD:193:VAL:O    | 26:DD:193:VAL:HG23 | 2.11                     | 0.49              |
| 27:DE:193:VAL:HG12 | 27:DE:199:MET:H    | 1.76                     | 0.49              |
| 28:DF:107:VAL:N    | 28:DF:108:PRO:HD2  | 2.26                     | 0.49              |
| 28:DF:115:GLY:HA3  | 28:DF:177:ARG:HB2  | 1.94                     | 0.49              |
| 29:DG:53:PRO:HG2   | 29:DG:61:TRP:HZ3   | 1.72                     | 0.49              |
| 32:DK:53:LYS:O     | 32:DK:56:ASP:HB2   | 2.12                     | 0.49              |
| 35:DN:58:ASP:O     | 35:DN:62:ASN:HB2   | 2.10                     | 0.49              |
| 37:DP:26:GLU:CD    | 37:DP:46:VAL:HG13  | 2.37                     | 0.49              |
| 42:DU:10:VAL:O     | 42:DU:21:ARG:HA    | 2.12                     | 0.49              |
| 48:D1:9:LYS:HG2    | 48:D1:24:LYS:HG2   | 1.93                     | 0.49              |
| 49:D2:12:ARG:CG    | 49:D2:46:LYS:HA    | 2.42                     | 0.49              |
| 1:AA:189:A:H2'     | 1:AA:190:A:C8      | 2.47                     | 0.49              |
| 1:AA:399:G:H2'     | 1:AA:400:C:H6      | 1.77                     | 0.49              |
| 1:AA:1363:A:N3     | 1:AA:1363:A:H2'    | 2.27                     | 0.49              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:AC:151:GLU:HB2   | 2:AC:200:TRP:HZ3  | 1.75                     | 0.49              |
| 3:AD:98:ASP:CG     | 3:AD:132:ALA:HB1  | 2.36                     | 0.49              |
| 5:AF:38:ARG:HH21   | 5:AF:96:VAL:HG12  | 1.77                     | 0.49              |
| 7:AH:49:LYS:HG3    | 7:AH:50:VAL:N     | 2.25                     | 0.49              |
| 7:AH:98:LEU:H      | 7:AH:98:LEU:HD12  | 1.77                     | 0.49              |
| 8:AI:23:GLY:O      | 8:AI:61:ASP:HB2   | 2.12                     | 0.49              |
| 10:AK:88:PRO:HA    | 10:AK:92:ARG:NE   | 2.27                     | 0.49              |
| 17:AR:46:THR:CG2   | 17:AR:51:GLN:HB2  | 2.42                     | 0.49              |
| 20:AB:41:ASN:ND2   | 20:AB:44:LYS:HE2  | 2.26                     | 0.49              |
| 20:AB:111:LYS:O    | 20:AB:114:LYS:HB2 | 2.11                     | 0.49              |
| 20:AB:202:ASN:HD22 | 20:AB:204:ASP:N   | 1.99                     | 0.49              |
| 23:BB:773:U:H4'    | 25:BC:47:ARG:CB   | 2.41                     | 0.49              |
| 23:BB:898:C:H2'    | 23:BB:899:A:C8    | 2.46                     | 0.49              |
| 23:BB:1051:G:H2'   | 23:BB:1052:C:C6   | 2.47                     | 0.49              |
| 23:BB:1082:U:C4    | 23:BB:1086:A:N1   | 2.79                     | 0.49              |
| 23:BB:2026:U:H2'   | 23:BB:2027:G:H8   | 1.78                     | 0.49              |
| 23:BB:2240:U:O2'   | 23:BB:2241:A:H5'  | 2.12                     | 0.49              |
| 23:BB:2502:G:H5'   | 23:BB:2503:A:C5'  | 2.36                     | 0.49              |
| 23:BB:2514:U:H2'   | 23:BB:2515:C:H6   | 1.77                     | 0.49              |
| 25:BC:30:ALA:H     | 25:BC:31:PRO:CD   | 2.12                     | 0.49              |
| 25:BC:208:GLY:C    | 25:BC:210:ALA:H   | 2.20                     | 0.49              |
| 26:BD:7:LYS:HD3    | 26:BD:197:THR:H   | 1.76                     | 0.49              |
| 26:BD:84:LEU:O     | 26:BD:84:LEU:HG   | 2.12                     | 0.49              |
| 26:BD:126:ASN:O    | 26:BD:127:PHE:CB  | 2.50                     | 0.49              |
| 26:BD:142:VAL:C    | 26:BD:144:GLY:N   | 2.67                     | 0.49              |
| 29:BG:16:VAL:HG12  | 29:BG:17:LYS:N    | 2.27                     | 0.49              |
| 29:BG:17:LYS:HB3   | 29:BG:24:THR:CG2  | 2.42                     | 0.49              |
| 32:BK:33:ALA:HB3   | 32:BK:39:ILE:HD11 | 1.94                     | 0.49              |
| 33:BL:56:PRO:HA    | 33:BL:60:ARG:CZ   | 2.41                     | 0.49              |
| 33:BL:111:ILE:HD13 | 33:BL:111:ILE:N   | 2.26                     | 0.49              |
| 35:BN:125:ALA:HA   | 47:B0:51:ARG:HH12 | 1.77                     | 0.49              |
| 36:BO:87:ILE:HG22  | 36:BO:114:GLY:HA2 | 1.94                     | 0.49              |
| 37:BP:36:LYS:HD3   | 37:BP:37:LYS:H    | 1.76                     | 0.49              |
| 38:BQ:112:ALA:HA   | 38:BQ:115:ALA:HB3 | 1.94                     | 0.49              |
| 40:BS:86:MET:O     | 40:BS:94:ASP:HB3  | 2.12                     | 0.49              |
| 41:BT:66:LYS:H     | 41:BT:77:ARG:HA   | 1.77                     | 0.49              |
| 43:BW:30:VAL:HG12  | 43:BW:31:LEU:N    | 2.27                     | 0.49              |
| 52:BI:96:LYS:N     | 52:BI:96:LYS:HD2  | 2.27                     | 0.49              |
| 1:CA:189:A:H2'     | 1:CA:190:A:C8     | 2.47                     | 0.49              |
| 1:CA:1121:U:H2'    | 1:CA:1122:U:C6    | 2.47                     | 0.49              |
| 1:CA:1285:A:O2'    | 1:CA:1286:U:H2'   | 2.12                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:CC:52:SER:HA     | 2:CC:114:LEU:HG    | 1.95                     | 0.49              |
| 6:CG:107:ALA:HB1   | 6:CG:115:MET:HE1   | 1.94                     | 0.49              |
| 7:CH:29:SER:O      | 7:CH:30:LYS:C      | 2.55                     | 0.49              |
| 10:CK:17:ASP:CG    | 10:CK:36:ARG:HH11  | 2.19                     | 0.49              |
| 10:CK:86:LYS:HB2   | 10:CK:112:VAL:HG23 | 1.94                     | 0.49              |
| 12:CM:2:ARG:HB3    | 12:CM:6:ILE:H      | 1.77                     | 0.49              |
| 12:CM:15:VAL:HG13  | 12:CM:40:GLU:CB    | 2.43                     | 0.49              |
| 15:CP:32:PHE:C     | 15:CP:32:PHE:HD1   | 2.20                     | 0.49              |
| 20:CB:130:LYS:HE2  | 20:CB:133:ALA:HB3  | 1.94                     | 0.49              |
| 23:DB:160:A:N6     | 23:DB:167:A:H1'    | 2.26                     | 0.49              |
| 23:DB:455:C:C4     | 23:DB:472:A:H2'    | 2.47                     | 0.49              |
| 23:DB:572:A:H5''   | 23:DB:573:U:OP2    | 2.12                     | 0.49              |
| 23:DB:1039:A:H2'   | 23:DB:1040:A:H8    | 1.75                     | 0.49              |
| 23:DB:1099:G:C5'   | 52:DI:4:VAL:HG12   | 2.42                     | 0.49              |
| 23:DB:1309:G:H4'   | 49:D2:7:PRO:CB     | 2.41                     | 0.49              |
| 23:DB:1747:U:H2'   | 23:DB:1748:C:C6    | 2.47                     | 0.49              |
| 23:DB:2080:A:H2'   | 23:DB:2081:U:H6    | 1.76                     | 0.49              |
| 23:DB:2240:U:O2'   | 23:DB:2241:A:H5'   | 2.11                     | 0.49              |
| 23:DB:2294:G:OP1   | 36:DO:9:ARG:HG3    | 2.12                     | 0.49              |
| 24:DV:76:ASP:H     | 24:DV:90:ASP:HB2   | 1.77                     | 0.49              |
| 25:DC:220:ARG:HA   | 25:DC:220:ARG:NH1  | 2.27                     | 0.49              |
| 26:DD:124:ARG:HH11 | 26:DD:124:ARG:HB3  | 1.77                     | 0.49              |
| 29:DG:84:LYS:O     | 29:DG:132:LEU:HG   | 2.12                     | 0.49              |
| 33:DL:92:LEU:HA    | 33:DL:96:LYS:CG    | 2.41                     | 0.49              |
| 35:DN:14:SER:HA    | 35:DN:17:ARG:NH1   | 2.27                     | 0.49              |
| 35:DN:112:TYR:O    | 35:DN:113:ILE:HB   | 2.12                     | 0.49              |
| 39:DR:46:GLU:HG3   | 39:DR:51:VAL:HG21  | 1.95                     | 0.49              |
| 43:DW:42:THR:OG1   | 43:DW:65:LYS:HA    | 2.12                     | 0.49              |
| 49:D2:12:ARG:HG2   | 49:D2:46:LYS:HA    | 1.94                     | 0.49              |
| 50:D3:34:LYS:HD2   | 50:D3:34:LYS:N     | 2.26                     | 0.49              |
| 1:AA:114:U:H2'     | 1:AA:115:G:C8      | 2.47                     | 0.49              |
| 1:AA:123:U:H5''    | 1:AA:311:C:O2'     | 2.12                     | 0.49              |
| 1:AA:314:C:O2'     | 1:AA:315:A:H5'     | 2.12                     | 0.49              |
| 1:AA:947:G:H2'     | 1:AA:948:C:H6      | 1.76                     | 0.49              |
| 1:AA:1018:G:H2'    | 1:AA:1019:A:C8     | 2.47                     | 0.49              |
| 1:AA:1437:A:H2'    | 1:AA:1438:G:H8     | 1.77                     | 0.49              |
| 2:AC:122:GLN:O     | 2:AC:127:VAL:HG22  | 2.12                     | 0.49              |
| 2:AC:135:ARG:C     | 2:AC:137:VAL:H     | 2.20                     | 0.49              |
| 4:AE:73:VAL:HG12   | 4:AE:74:ALA:N      | 2.27                     | 0.49              |
| 6:AG:49:LEU:HB2    | 6:AG:57:GLU:HG3    | 1.94                     | 0.49              |
| 7:AH:17:GLN:HE21   | 7:AH:62:LEU:HG     | 1.76                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:AI:62:LEU:N      | 8:AI:62:LEU:HD22  | 2.26                     | 0.49              |
| 14:AO:27:GLN:O     | 14:AO:31:LEU:HD23 | 2.12                     | 0.49              |
| 19:AT:66:ILE:HG23  | 19:AT:70:LYS:HD3  | 1.94                     | 0.49              |
| 20:AB:23:ASN:C     | 20:AB:23:ASN:HD22 | 2.20                     | 0.49              |
| 20:AB:101:THR:HG23 | 20:AB:102:ASN:N   | 2.28                     | 0.49              |
| 23:BB:184:C:H2'    | 23:BB:185:G:C8    | 2.48                     | 0.49              |
| 23:BB:592:A:H2'    | 23:BB:593:U:C6    | 2.47                     | 0.49              |
| 23:BB:663:G:OP1    | 33:BL:27:LEU:HD11 | 2.12                     | 0.49              |
| 23:BB:1151:A:H2'   | 23:BB:1152:C:C6   | 2.47                     | 0.49              |
| 23:BB:1681:G:H2'   | 23:BB:1757:A:N1   | 2.27                     | 0.49              |
| 23:BB:2247:A:H2'   | 23:BB:2248:C:H6   | 1.77                     | 0.49              |
| 23:BB:2249:U:H4'   | 23:BB:2275:C:C5   | 2.47                     | 0.49              |
| 23:BB:2412:A:H2'   | 23:BB:2413:G:O4'  | 2.11                     | 0.49              |
| 23:BB:2648:G:H2'   | 23:BB:2649:C:C6   | 2.47                     | 0.49              |
| 23:BB:2724:U:OP1   | 26:BD:116:LYS:HD2 | 2.12                     | 0.49              |
| 24:BV:26:PHE:CE2   | 24:BV:44:HIS:HA   | 2.47                     | 0.49              |
| 26:BD:17:GLU:HA    | 37:BP:80:VAL:HG21 | 1.95                     | 0.49              |
| 26:BD:25:THR:HB    | 37:BP:5:LYS:HZ3   | 1.77                     | 0.49              |
| 26:BD:128:ARG:HH11 | 26:BD:144:GLY:HA2 | 1.77                     | 0.49              |
| 28:BF:18:GLU:O     | 28:BF:19:PHE:CB   | 2.59                     | 0.49              |
| 28:BF:41:GLU:HG3   | 28:BF:49:LEU:HD12 | 1.94                     | 0.49              |
| 31:BJ:56:VAL:HG12  | 31:BJ:57:LEU:H    | 1.77                     | 0.49              |
| 31:BJ:72:LYS:O     | 31:BJ:74:TYR:N    | 2.46                     | 0.49              |
| 31:BJ:103:ILE:HG22 | 31:BJ:103:ILE:O   | 2.12                     | 0.49              |
| 33:BL:123:ARG:HH22 | 33:BL:141:LYS:NZ  | 2.10                     | 0.49              |
| 34:BM:89:VAL:HG22  | 34:BM:89:VAL:O    | 2.12                     | 0.49              |
| 39:BR:65:ALA:O     | 39:BR:66:HIS:HB2  | 2.12                     | 0.49              |
| 39:BR:85:LYS:O     | 39:BR:85:LYS:HG3  | 2.12                     | 0.49              |
| 41:BT:8:LEU:CB     | 44:BX:19:LEU:HD11 | 2.32                     | 0.49              |
| 41:BT:69:ARG:N     | 41:BT:75:GLY:HA3  | 2.28                     | 0.49              |
| 1:CA:418:C:H2'     | 1:CA:419:C:H6     | 1.78                     | 0.49              |
| 1:CA:626:G:H2'     | 1:CA:627:G:C8     | 2.48                     | 0.49              |
| 1:CA:1229:A:H2'    | 1:CA:1230:C:C6    | 2.47                     | 0.49              |
| 1:CA:1343:G:H2'    | 1:CA:1344:C:H6    | 1.78                     | 0.49              |
| 2:CC:17:TRP:C      | 2:CC:19:SER:H     | 2.20                     | 0.49              |
| 2:CC:88:LYS:O      | 2:CC:88:LYS:HE3   | 2.13                     | 0.49              |
| 12:CM:79:LEU:HD22  | 12:CM:86:ARG:NE   | 2.27                     | 0.49              |
| 12:CM:95:PRO:HB2   | 12:CM:99:GLN:OE1  | 2.11                     | 0.49              |
| 13:CN:61:ASN:HB2   | 13:CN:72:PHE:CZ   | 2.47                     | 0.49              |
| 15:CP:22:ALA:HA    | 15:CP:33:ILE:HG13 | 1.95                     | 0.49              |
| 15:CP:78:VAL:O     | 15:CP:78:VAL:HG13 | 2.12                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:CQ:13:SER:O     | 16:CQ:20:ILE:HG13  | 2.13                     | 0.49              |
| 16:CQ:56:ASP:HA    | 16:CQ:81:ALA:CA    | 2.42                     | 0.49              |
| 23:DB:335:C:O2'    | 23:DB:336:C:H5'    | 2.12                     | 0.49              |
| 23:DB:398:C:OP1    | 46:DZ:49:ARG:NH1   | 2.45                     | 0.49              |
| 23:DB:521:U:H2'    | 23:DB:522:A:H8     | 1.76                     | 0.49              |
| 23:DB:764:A:H5''   | 25:DC:208:GLY:CA   | 2.42                     | 0.49              |
| 23:DB:1038:G:H2'   | 23:DB:1039:A:H8    | 1.76                     | 0.49              |
| 23:DB:1152:C:O2'   | 23:DB:1153:C:H5'   | 2.11                     | 0.49              |
| 23:DB:1299:G:C4'   | 23:DB:1301:A:H1'   | 2.40                     | 0.49              |
| 23:DB:2244:U:H1'   | 23:DB:2434:A:C4    | 2.48                     | 0.49              |
| 23:DB:2776:A:H4'   | 23:DB:2777:G:O5'   | 2.13                     | 0.49              |
| 23:DB:2803:G:H2'   | 23:DB:2804:U:C6    | 2.47                     | 0.49              |
| 23:DB:2876:G:H4'   | 37:DP:2:ASN:HB3    | 1.93                     | 0.49              |
| 26:DD:148:GLN:HB3  | 26:DD:151:THR:HG23 | 1.95                     | 0.49              |
| 27:DE:127:GLU:CA   | 27:DE:157:LEU:HD13 | 2.32                     | 0.49              |
| 28:DF:125:GLY:O    | 28:DF:157:THR:HB   | 2.13                     | 0.49              |
| 30:DH:54:LEU:O     | 30:DH:58:LEU:HD23  | 2.12                     | 0.49              |
| 31:DJ:89:PHE:CD1   | 31:DJ:92:MET:HE2   | 2.47                     | 0.49              |
| 31:DJ:90:GLU:O     | 31:DJ:93:ILE:HG13  | 2.12                     | 0.49              |
| 32:DK:99:ILE:HD12  | 32:DK:118:LEU:HD12 | 1.94                     | 0.49              |
| 33:DL:108:ALA:HB1  | 33:DL:125:LEU:HD13 | 1.94                     | 0.49              |
| 34:DM:20:LEU:HD22  | 34:DM:38:ARG:HG2   | 1.94                     | 0.49              |
| 34:DM:71:LYS:O     | 34:DM:73:ILE:N     | 2.45                     | 0.49              |
| 34:DM:119:LEU:HD22 | 34:DM:119:LEU:H    | 1.78                     | 0.49              |
| 35:DN:5:LYS:HA     | 35:DN:5:LYS:CE     | 2.34                     | 0.49              |
| 36:DO:1:MET:HE3    | 36:DO:1:MET:O      | 2.13                     | 0.49              |
| 36:DO:45:SER:C     | 36:DO:47:VAL:H     | 2.20                     | 0.49              |
| 40:DS:24:ILE:HG23  | 40:DS:35:ILE:HG21  | 1.93                     | 0.49              |
| 42:DU:66:VAL:HG13  | 42:DU:67:SER:N     | 2.27                     | 0.49              |
| 43:DW:65:LYS:HB2   | 43:DW:65:LYS:HZ2   | 1.77                     | 0.49              |
| 45:DY:23:LEU:HD13  | 45:DY:28:LEU:HD23  | 1.94                     | 0.49              |
| 45:DY:43:ILE:HD11  | 45:DY:47:ILE:HD11  | 1.94                     | 0.49              |
| 47:D0:12:ARG:NH2   | 47:D0:16:ARG:HG3   | 2.27                     | 0.49              |
| 52:DI:19:PRO:HB2   | 52:DI:22:PRO:HD2   | 1.93                     | 0.49              |
| 52:DI:63:ASP:OD1   | 52:DI:65:SER:HB2   | 2.12                     | 0.49              |
| 1:AA:182:A:H1'     | 1:AA:183:C:C5      | 2.48                     | 0.49              |
| 1:AA:205:A:H2'     | 1:AA:206:C:C6      | 2.44                     | 0.49              |
| 1:AA:317:U:H2'     | 1:AA:318:G:C8      | 2.47                     | 0.49              |
| 1:AA:366:A:O2'     | 1:AA:367:U:P       | 2.70                     | 0.49              |
| 1:AA:576:C:H3'     | 1:AA:576:C:OP2     | 2.12                     | 0.49              |
| 1:AA:662:U:O2'     | 1:AA:836:G:H5''    | 2.12                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1048:G:H4'   | 13:AN:2:LYS:HZ1    | 1.76                     | 0.49              |
| 2:AC:143:LEU:HD22 | 2:AC:143:LEU:H     | 1.76                     | 0.49              |
| 5:AF:39:LEU:HD13  | 5:AF:40:GLU:H      | 1.77                     | 0.49              |
| 7:AH:39:LEU:HB2   | 7:AH:45:ILE:CD1    | 2.43                     | 0.49              |
| 8:AI:32:ARG:HD3   | 8:AI:37:TYR:HD1    | 1.75                     | 0.49              |
| 15:AP:29:ASN:HD22 | 15:AP:29:ASN:N     | 2.11                     | 0.49              |
| 18:AS:35:ARG:HG2  | 18:AS:50:VAL:HG13  | 1.94                     | 0.49              |
| 22:BA:74:U:H2'    | 22:BA:75:G:O4'     | 2.12                     | 0.49              |
| 23:BB:38:A:H1'    | 27:BE:44:ARG:HA    | 1.93                     | 0.49              |
| 23:BB:650:C:O3'   | 50:B3:16:THR:HB    | 2.12                     | 0.49              |
| 23:BB:836:G:H2'   | 23:BB:837:C:H6     | 1.77                     | 0.49              |
| 23:BB:1169:A:O2'  | 23:BB:1170:C:H5'   | 2.12                     | 0.49              |
| 23:BB:1684:G:H2'  | 23:BB:1685:C:H6    | 1.77                     | 0.49              |
| 23:BB:2528:U:O2'  | 23:BB:2529:G:H3'   | 2.13                     | 0.49              |
| 23:BB:2590:A:H2'  | 23:BB:2591:C:H6    | 1.76                     | 0.49              |
| 25:BC:209:ALA:HA  | 25:BC:213:ARG:CZ   | 2.43                     | 0.49              |
| 26:BD:4:LEU:H     | 26:BD:4:LEU:HD23   | 1.77                     | 0.49              |
| 31:BJ:15:TRP:HB3  | 31:BJ:53:TYR:CD2   | 2.48                     | 0.49              |
| 34:BM:7:THR:C     | 34:BM:8:LYS:HD3    | 2.37                     | 0.49              |
| 37:BP:5:LYS:C     | 37:BP:7:LEU:N      | 2.71                     | 0.49              |
| 38:BQ:27:ARG:N    | 38:BQ:32:ARG:HH21  | 2.11                     | 0.49              |
| 38:BQ:77:LYS:HB3  | 38:BQ:116:LEU:HD11 | 1.93                     | 0.49              |
| 41:BT:16:VAL:HG22 | 41:BT:16:VAL:O     | 2.13                     | 0.49              |
| 46:BZ:5:ILE:HG23  | 46:BZ:63:ARG:NE    | 2.27                     | 0.49              |
| 47:B0:29:VAL:HG13 | 47:B0:30:ASP:N     | 2.26                     | 0.49              |
| 52:BI:116:MET:SD  | 52:BI:124:MET:HB2  | 2.52                     | 0.49              |
| 1:CA:8:A:C5       | 3:CD:205:LYS:HA    | 2.47                     | 0.49              |
| 1:CA:272:C:H2'    | 1:CA:273:U:C6      | 2.47                     | 0.49              |
| 1:CA:712:A:O2'    | 1:CA:713:G:H5'     | 2.12                     | 0.49              |
| 1:CA:1031:C:H5'   | 1:CA:1032:G:N9     | 2.28                     | 0.49              |
| 1:CA:1121:U:O2'   | 1:CA:1122:U:H5'    | 2.13                     | 0.49              |
| 1:CA:1237:C:OP1   | 1:CA:1238:A:H1'    | 2.11                     | 0.49              |
| 1:CA:1243:C:H2'   | 1:CA:1244:G:C8     | 2.48                     | 0.49              |
| 1:CA:1526:G:O5'   | 21:CU:38:GLU:HB2   | 2.12                     | 0.49              |
| 4:CE:81:GLN:NE2   | 4:CE:148:SER:HA    | 2.26                     | 0.49              |
| 4:CE:89:THR:C     | 4:CE:91:SER:H      | 2.18                     | 0.49              |
| 4:CE:114:LEU:HD13 | 4:CE:122:VAL:HG21  | 1.94                     | 0.49              |
| 5:CF:18:VAL:O     | 5:CF:22:ILE:HG13   | 2.13                     | 0.49              |
| 5:CF:85:ILE:HG22  | 5:CF:86:ARG:N      | 2.27                     | 0.49              |
| 7:CH:10:LEU:HD11  | 7:CH:126:CYS:SG    | 2.52                     | 0.49              |
| 12:CM:80:MET:HA   | 12:CM:87:GLY:HA3   | 1.94                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 14:CO:25:GLU:OE2   | 14:CO:76:ARG:HD3  | 2.12                     | 0.49              |
| 16:CQ:58:VAL:HB    | 16:CQ:74:LEU:HD23 | 1.94                     | 0.49              |
| 20:CB:67:LEU:HD22  | 20:CB:157:PRO:HG3 | 1.94                     | 0.49              |
| 22:DA:63:C:H2'     | 22:DA:64:G:H8     | 1.77                     | 0.49              |
| 23:DB:41:C:O2'     | 23:DB:42:A:H5'    | 2.13                     | 0.49              |
| 23:DB:244:A:H2'    | 23:DB:245:G:O4'   | 2.12                     | 0.49              |
| 23:DB:536:G:C5'    | 38:DQ:52:ARG:NH2  | 2.75                     | 0.49              |
| 23:DB:592:A:H2'    | 23:DB:593:U:C6    | 2.47                     | 0.49              |
| 23:DB:1199:U:O2'   | 38:DQ:2:ARG:CB    | 2.60                     | 0.49              |
| 23:DB:2047:C:O2'   | 23:DB:2048:G:H5'  | 2.12                     | 0.49              |
| 23:DB:2314:A:H2'   | 23:DB:2315:G:H8   | 1.77                     | 0.49              |
| 23:DB:2393:U:H4'   | 33:DL:60:ARG:O    | 2.12                     | 0.49              |
| 23:DB:2425:A:O2'   | 23:DB:2426:A:OP2  | 2.28                     | 0.49              |
| 23:DB:2654:A:N1    | 23:DB:2665:A:H5'' | 2.27                     | 0.49              |
| 23:DB:2743:U:H2'   | 23:DB:2744:G:C5'  | 2.40                     | 0.49              |
| 23:DB:2860:A:H2'   | 23:DB:2861:U:O4'  | 2.12                     | 0.49              |
| 25:DC:37:SER:HB2   | 25:DC:62:ARG:HG3  | 1.94                     | 0.49              |
| 27:DE:191:ASP:HA   | 27:DE:194:LYS:NZ  | 2.27                     | 0.49              |
| 28:DF:141:ASP:C    | 28:DF:143:ASP:H   | 2.21                     | 0.49              |
| 29:DG:17:LYS:O     | 29:DG:17:LYS:HE3  | 2.12                     | 0.49              |
| 33:DL:18:ARG:NH1   | 33:DL:21:ARG:HD3  | 2.26                     | 0.49              |
| 33:DL:62:PRO:HG3   | 50:D3:12:ARG:CZ   | 2.43                     | 0.49              |
| 34:DM:5:LYS:HG2    | 34:DM:68:PHE:HE1  | 1.78                     | 0.49              |
| 38:DQ:92:LYS:C     | 38:DQ:93:ILE:HG23 | 2.36                     | 0.49              |
| 39:DR:69:GLY:HA2   | 39:DR:96:VAL:HG13 | 1.94                     | 0.49              |
| 40:DS:103:ILE:O    | 40:DS:104:THR:HB  | 2.11                     | 0.49              |
| 41:DT:67:VAL:HG12  | 41:DT:68:LYS:N    | 2.26                     | 0.49              |
| 44:DX:18:LEU:O     | 44:DX:22:LEU:HB2  | 2.13                     | 0.49              |
| 44:DX:22:LEU:HB3   | 44:DX:25:GLN:OE1  | 2.12                     | 0.49              |
| 48:D1:34:GLU:HG2   | 48:D1:50:GLU:OE1  | 2.11                     | 0.49              |
| 1:AA:997:U:H2'     | 1:AA:998:C:C6     | 2.46                     | 0.49              |
| 1:AA:1221:G:O3'    | 18:AS:76:THR:HG21 | 2.12                     | 0.49              |
| 1:AA:1386:G:O2'    | 1:AA:1387:G:H5'   | 2.12                     | 0.49              |
| 4:AE:87:VAL:CG1    | 4:AE:92:ARG:HD3   | 2.42                     | 0.49              |
| 8:AI:56:MET:HA     | 8:AI:59:LYS:NZ    | 2.22                     | 0.49              |
| 10:AK:85:VAL:O     | 10:AK:111:ASP:HA  | 2.12                     | 0.49              |
| 12:AM:53:ASP:HA    | 12:AM:56:ARG:HD2  | 1.93                     | 0.49              |
| 14:AO:66:LEU:HB3   | 14:AO:77:TYR:HE1  | 1.77                     | 0.49              |
| 14:AO:68:TYR:CE1   | 14:AO:72:LYS:HE3  | 2.47                     | 0.49              |
| 20:AB:119:GLN:HE22 | 20:AB:127:LYS:HD3 | 1.77                     | 0.49              |
| 23:BB:69:C:H2'     | 23:BB:70:G:C8     | 2.47                     | 0.49              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:635:C:H3'   | 33:BL:109:LYS:HZ1  | 1.76                     | 0.49              |
| 23:BB:1255:U:O2'  | 27:BE:67:ARG:HB3   | 2.12                     | 0.49              |
| 23:BB:1501:G:O2'  | 23:BB:1502:A:H5'   | 2.12                     | 0.49              |
| 23:BB:2000:C:OP1  | 35:BN:2:ARG:NE     | 2.45                     | 0.49              |
| 23:BB:2082:A:O2'  | 23:BB:2083:G:H5'   | 2.13                     | 0.49              |
| 23:BB:2249:U:H4'  | 23:BB:2275:C:H5    | 1.76                     | 0.49              |
| 23:BB:2314:A:H2'  | 23:BB:2315:G:C8    | 2.47                     | 0.49              |
| 23:BB:2831:G:O4'  | 23:BB:2883:A:C2    | 2.65                     | 0.49              |
| 25:BC:12:ARG:HB3  | 25:BC:18:VAL:HB    | 1.94                     | 0.49              |
| 25:BC:66:PHE:HE2  | 25:BC:104:LEU:HD21 | 1.77                     | 0.49              |
| 25:BC:204:LEU:CD1 | 25:BC:211:ARG:HH11 | 2.25                     | 0.49              |
| 26:BD:157:LYS:HE2 | 26:BD:157:LYS:HA   | 1.94                     | 0.49              |
| 27:BE:154:ASP:OD1 | 27:BE:156:ASN:HB2  | 2.13                     | 0.49              |
| 28:BF:90:LEU:O    | 28:BF:95:MET:HG3   | 2.12                     | 0.49              |
| 28:BF:176:PHE:O   | 28:BF:177:ARG:HB3  | 2.11                     | 0.49              |
| 29:BG:6:ALA:HB3   | 29:BG:7:PRO:HD3    | 1.93                     | 0.49              |
| 31:BJ:17:VAL:HG22 | 31:BJ:55:ILE:CG2   | 2.42                     | 0.49              |
| 34:BM:62:LYS:CB   | 34:BM:104:GLU:HB2  | 2.42                     | 0.49              |
| 34:BM:67:VAL:HG21 | 34:BM:95:LEU:HD11  | 1.94                     | 0.49              |
| 43:BW:16:GLU:HG3  | 43:BW:37:VAL:HG22  | 1.93                     | 0.49              |
| 43:BW:43:LYS:HG2  | 43:BW:76:ARG:NE    | 2.25                     | 0.49              |
| 44:BX:1:MET:HE3   | 44:BX:1:MET:N      | 2.27                     | 0.49              |
| 44:BX:19:LEU:H    | 44:BX:19:LEU:HD12  | 1.77                     | 0.49              |
| 1:CA:33:A:H2'     | 1:CA:34:C:H6       | 1.77                     | 0.49              |
| 1:CA:219:U:H2'    | 1:CA:220:G:H8      | 1.77                     | 0.49              |
| 1:CA:1054:C:H1'   | 1:CA:1196:A:C5     | 2.48                     | 0.49              |
| 1:CA:1162:C:H2'   | 1:CA:1163:A:C8     | 2.47                     | 0.49              |
| 1:CA:1163:A:H2'   | 1:CA:1164:G:C8     | 2.46                     | 0.49              |
| 1:CA:1238:A:H2    | 1:CA:1241:G:N3     | 2.10                     | 0.49              |
| 3:CD:96:ARG:O     | 3:CD:99:ASN:HB3    | 2.12                     | 0.49              |
| 3:CD:106:PHE:HD1  | 3:CD:158:LEU:HD21  | 1.78                     | 0.49              |
| 4:CE:88:HIS:CE1   | 4:CE:137:ARG:HG2   | 2.48                     | 0.49              |
| 5:CF:42:TRP:NE1   | 5:CF:61:LEU:HD23   | 2.27                     | 0.49              |
| 9:CJ:102:LEU:N    | 9:CJ:102:LEU:HD22  | 2.27                     | 0.49              |
| 10:CK:112:VAL:HA  | 17:CR:72:ARG:HD3   | 1.94                     | 0.49              |
| 12:CM:22:TYR:HB3  | 12:CM:69:ARG:NH2   | 2.27                     | 0.49              |
| 12:CM:78:ARG:HG3  | 28:DF:111:ARG:NH1  | 2.26                     | 0.49              |
| 12:CM:96:VAL:C    | 12:CM:98:GLY:H     | 2.20                     | 0.49              |
| 23:DB:15:G:O2'    | 23:DB:16:C:H5'     | 2.13                     | 0.49              |
| 23:DB:21:A:H2'    | 23:DB:22:C:C6      | 2.48                     | 0.49              |
| 23:DB:378:C:O2'   | 23:DB:379:G:H5'    | 2.12                     | 0.49              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DB:587:C:H4'   | 23:DB:588:U:C6    | 2.48                     | 0.49              |
| 23:DB:721:A:H2'   | 23:DB:722:A:C8    | 2.48                     | 0.49              |
| 23:DB:827:U:H5'   | 23:DB:828:U:O5'   | 2.12                     | 0.49              |
| 23:DB:1135:C:N4   | 23:DB:1139:G:C6   | 2.81                     | 0.49              |
| 23:DB:2377:A:C2   | 36:DO:92:PHE:HE1  | 2.30                     | 0.49              |
| 23:DB:2528:U:O2'  | 23:DB:2529:G:H3'  | 2.13                     | 0.49              |
| 25:DC:86:ARG:O    | 25:DC:86:ARG:HG3  | 2.12                     | 0.49              |
| 27:DE:46:GLN:HG3  | 27:DE:49:ARG:NH2  | 2.28                     | 0.49              |
| 27:DE:188:MET:HE1 | 27:DE:190:ALA:HB2 | 1.94                     | 0.49              |
| 28:DF:40:GLY:H    | 28:DF:84:ILE:CG2  | 2.26                     | 0.49              |
| 30:DH:53:GLU:CD   | 30:DH:57:LYS:HD2  | 2.37                     | 0.49              |
| 30:DH:125:THR:HA  | 30:DH:146:VAL:CB  | 2.32                     | 0.49              |
| 32:DK:64:ARG:O    | 32:DK:65:THR:HG23 | 2.13                     | 0.49              |
| 33:DL:77:ILE:CG2  | 33:DL:92:LEU:HG   | 2.42                     | 0.49              |
| 43:DW:42:THR:HG22 | 43:DW:67:LYS:O    | 2.13                     | 0.49              |
| 43:DW:76:ARG:C    | 43:DW:78:PHE:H    | 2.20                     | 0.49              |
| 47:D0:11:LYS:O    | 47:D0:15:ARG:HB2  | 2.13                     | 0.49              |
| 48:D1:29:LYS:CB   | 48:D1:30:PRO:HD3  | 2.17                     | 0.49              |
| 51:D4:3:VAL:CG1   | 51:D4:4:ARG:H     | 2.13                     | 0.49              |
| 1:AA:35:G:H2'     | 1:AA:36:C:H6      | 1.78                     | 0.49              |
| 1:AA:301:G:H2'    | 1:AA:302:G:C8     | 2.48                     | 0.49              |
| 1:AA:382:A:H2'    | 1:AA:383:A:C8     | 2.48                     | 0.49              |
| 1:AA:724:G:O2'    | 1:AA:725:G:H5'    | 2.11                     | 0.49              |
| 1:AA:1492:A:H2'   | 1:AA:1493:A:O4'   | 2.12                     | 0.49              |
| 8:AI:24:ASN:O     | 8:AI:61:ASP:HA    | 2.12                     | 0.49              |
| 10:AK:69:CYS:O    | 10:AK:73:VAL:HG23 | 2.12                     | 0.49              |
| 11:AL:34:THR:HG21 | 11:AL:53:ARG:CZ   | 2.43                     | 0.49              |
| 16:AQ:19:SER:O    | 16:AQ:20:ILE:HG23 | 2.12                     | 0.49              |
| 23:BB:139:U:H5'   | 23:BB:140:C:C4    | 2.47                     | 0.49              |
| 23:BB:142:A:H1'   | 41:BT:2:ILE:HG21  | 1.93                     | 0.49              |
| 23:BB:1190:G:OP1  | 33:BL:41:ARG:CZ   | 2.60                     | 0.49              |
| 23:BB:1292:G:H2'  | 23:BB:1293:C:C6   | 2.48                     | 0.49              |
| 23:BB:1322:A:C2'  | 23:BB:1323:C:H5'  | 2.43                     | 0.49              |
| 23:BB:1562:U:H2'  | 23:BB:1563:U:C6   | 2.47                     | 0.49              |
| 23:BB:1727:C:H2'  | 23:BB:1728:C:H6   | 1.74                     | 0.49              |
| 23:BB:1881:C:H2'  | 23:BB:1882:U:O4'  | 2.13                     | 0.49              |
| 23:BB:1948:G:O2'  | 23:BB:1949:G:H5'  | 2.12                     | 0.49              |
| 23:BB:2287:A:OP1  | 23:BB:2287:A:H4'  | 2.10                     | 0.49              |
| 25:BC:70:LYS:HG2  | 25:BC:73:ILE:HD13 | 1.94                     | 0.49              |
| 26:BD:15:PHE:CD2  | 26:BD:18:ASP:HB2  | 2.47                     | 0.49              |
| 26:BD:83:ARG:HG2  | 26:BD:84:LEU:N    | 2.27                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 26:BD:170:VAL:HG11 | 26:BD:194:PRO:HB2 | 1.94                     | 0.49              |
| 28:BF:21:TYR:OH    | 28:BF:28:PRO:HD3  | 2.13                     | 0.49              |
| 28:BF:41:GLU:OE2   | 28:BF:48:LEU:HB3  | 2.13                     | 0.49              |
| 29:BG:40:VAL:CB    | 29:BG:63:GLN:HE22 | 2.25                     | 0.49              |
| 30:BH:80:ILE:HD12  | 30:BH:102:ALA:CB  | 2.43                     | 0.49              |
| 35:BN:102:PHE:N    | 35:BN:102:PHE:CD2 | 2.80                     | 0.49              |
| 37:BP:13:LYS:HA    | 37:BP:15:ASP:OD1  | 2.13                     | 0.49              |
| 38:BQ:63:ARG:HH11  | 38:BQ:63:ARG:CB   | 2.26                     | 0.49              |
| 40:BS:29:VAL:C     | 40:BS:31:GLN:N    | 2.69                     | 0.49              |
| 44:BX:18:LEU:HD12  | 44:BX:19:LEU:HD12 | 1.94                     | 0.49              |
| 44:BX:22:LEU:HD22  | 44:BX:26:PHE:N    | 2.23                     | 0.49              |
| 44:BX:30:MET:CG    | 44:BX:31:GLN:H    | 2.24                     | 0.49              |
| 44:BX:46:VAL:HG13  | 44:BX:47:ARG:N    | 2.28                     | 0.49              |
| 46:BZ:59:ARG:HB2   | 46:BZ:61:ASN:H    | 1.78                     | 0.49              |
| 1:CA:147:G:H2'     | 1:CA:148:G:C8     | 2.48                     | 0.49              |
| 1:CA:366:A:O2'     | 1:CA:367:U:P      | 2.70                     | 0.49              |
| 1:CA:662:U:O2'     | 1:CA:836:G:H5''   | 2.12                     | 0.49              |
| 1:CA:693:G:H2'     | 1:CA:694:A:O4'    | 2.12                     | 0.49              |
| 1:CA:1228:C:OP1    | 12:CM:112:ARG:HA  | 2.13                     | 0.49              |
| 2:CC:64:ARG:HA     | 2:CC:99:GLN:HB2   | 1.93                     | 0.49              |
| 3:CD:130:ASN:HD22  | 3:CD:130:ASN:N    | 2.06                     | 0.49              |
| 9:CJ:87:LEU:N      | 9:CJ:87:LEU:HD22  | 2.27                     | 0.49              |
| 10:CK:31:VAL:HG21  | 10:CK:66:ALA:HA   | 1.94                     | 0.49              |
| 22:DA:116:G:H4'    | 36:DO:54:VAL:CG2  | 2.42                     | 0.49              |
| 23:DB:185:G:H4'    | 23:DB:218:A:H4'   | 1.94                     | 0.49              |
| 23:DB:303:G:H2'    | 23:DB:304:U:C6    | 2.47                     | 0.49              |
| 23:DB:365:U:H2'    | 23:DB:366:C:O4'   | 2.12                     | 0.49              |
| 23:DB:465:G:H4'    | 49:D2:12:ARG:NH2  | 2.27                     | 0.49              |
| 23:DB:1082:U:H2'   | 23:DB:1083:U:O4'  | 2.12                     | 0.49              |
| 23:DB:1214:A:H2'   | 23:DB:1215:G:O4'  | 2.12                     | 0.49              |
| 23:DB:1256:G:H1'   | 27:DE:77:ILE:HD11 | 1.95                     | 0.49              |
| 23:DB:1292:G:H2'   | 23:DB:1293:C:C6   | 2.48                     | 0.49              |
| 23:DB:1881:C:H2'   | 23:DB:1882:U:O4'  | 2.12                     | 0.49              |
| 23:DB:1909:C:H2'   | 23:DB:1910:G:H8   | 1.77                     | 0.49              |
| 23:DB:1995:U:H1'   | 32:DK:3:GLN:HE22  | 1.78                     | 0.49              |
| 23:DB:2093:G:OP2   | 30:DH:23:ALA:HB3  | 2.12                     | 0.49              |
| 23:DB:2386:A:H4'   | 43:DW:38:ARG:HD3  | 1.94                     | 0.49              |
| 23:DB:2518:A:H2'   | 23:DB:2518:A:N3   | 2.26                     | 0.49              |
| 23:DB:2590:A:H2'   | 23:DB:2591:C:H6   | 1.76                     | 0.49              |
| 23:DB:2648:G:H2'   | 23:DB:2649:C:C6   | 2.47                     | 0.49              |
| 23:DB:2717:C:O2'   | 37:DP:95:LYS:HE3  | 2.13                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:DV:70:ILE:CD1   | 24:DV:71:LYS:H     | 2.23                     | 0.49              |
| 25:DC:143:VAL:O    | 25:DC:152:GLN:HB2  | 2.13                     | 0.49              |
| 27:DE:20:GLY:HA2   | 27:DE:106:LYS:HD2  | 1.95                     | 0.49              |
| 27:DE:46:GLN:CD    | 27:DE:86:ALA:HB3   | 2.38                     | 0.49              |
| 28:DF:116:LEU:HD22 | 28:DF:129:MET:HE1  | 1.94                     | 0.49              |
| 30:DH:81:ALA:HA    | 30:DH:147:VAL:O    | 2.12                     | 0.49              |
| 33:DL:108:ALA:O    | 33:DL:109:LYS:CB   | 2.61                     | 0.49              |
| 34:DM:11:LYS:O     | 34:DM:12:MET:HB2   | 2.13                     | 0.49              |
| 34:DM:42:THR:HG22  | 34:DM:45:GLN:NE2   | 2.27                     | 0.49              |
| 35:DN:35:LYS:HD3   | 35:DN:112:TYR:CE1  | 2.47                     | 0.49              |
| 38:DQ:89:ILE:HG22  | 38:DQ:90:ASP:N     | 2.26                     | 0.49              |
| 41:DT:26:LYS:O     | 41:DT:27:SER:HB3   | 2.13                     | 0.49              |
| 42:DU:10:VAL:HB    | 42:DU:68:ASN:ND2   | 2.27                     | 0.49              |
| 46:DZ:59:ARG:HA    | 46:DZ:62:LYS:HB2   | 1.94                     | 0.49              |
| 52:DI:7:TYR:HA     | 52:DI:59:THR:HA    | 1.95                     | 0.49              |
| 1:AA:693:G:H2'     | 1:AA:694:A:O4'     | 2.12                     | 0.49              |
| 1:AA:853:C:O2'     | 1:AA:854:U:H5'     | 2.12                     | 0.49              |
| 2:AC:11:LEU:HD13   | 2:AC:17:TRP:HE1    | 1.76                     | 0.49              |
| 8:AI:96:GLU:O      | 8:AI:99:LYS:HB3    | 2.12                     | 0.49              |
| 20:AB:57:ASN:HB2   | 20:AB:219:THR:HB   | 1.95                     | 0.49              |
| 20:AB:132:GLU:HG3  | 20:AB:136:ARG:HD2  | 1.94                     | 0.49              |
| 20:AB:139:GLU:HG2  | 20:AB:143:LEU:CD1  | 2.42                     | 0.49              |
| 21:AU:20:ARG:HG2   | 21:AU:20:ARG:O     | 2.13                     | 0.49              |
| 23:BB:25:U:OP1     | 40:BS:8:ARG:NH2    | 2.45                     | 0.49              |
| 23:BB:209:C:O2'    | 23:BB:210:C:H5'    | 2.12                     | 0.49              |
| 23:BB:600:G:H1'    | 27:BE:100:MET:HG3  | 1.95                     | 0.49              |
| 23:BB:991:C:H2'    | 23:BB:992:C:C6     | 2.47                     | 0.49              |
| 23:BB:1205:A:O2'   | 27:BE:164:LEU:HD21 | 2.13                     | 0.49              |
| 23:BB:1685:C:H2'   | 23:BB:1686:C:H6    | 1.78                     | 0.49              |
| 23:BB:1853:A:N1    | 23:BB:2087:G:H1'   | 2.27                     | 0.49              |
| 23:BB:2654:A:N1    | 23:BB:2665:A:H5''  | 2.27                     | 0.49              |
| 23:BB:2786:U:C4'   | 26:BD:66:GLY:HA2   | 2.43                     | 0.49              |
| 23:BB:2840:C:H2'   | 23:BB:2841:C:C6    | 2.48                     | 0.49              |
| 26:BD:13:ARG:O     | 26:BD:14:ILE:C     | 2.55                     | 0.49              |
| 26:BD:34:VAL:CA    | 26:BD:89:GLU:HB2   | 2.34                     | 0.49              |
| 26:BD:130:GLN:HE21 | 26:BD:138:LEU:HD12 | 1.71                     | 0.49              |
| 29:BG:139:VAL:O    | 29:BG:143:VAL:HG23 | 2.13                     | 0.49              |
| 30:BH:67:ALA:O     | 30:BH:71:LYS:HG3   | 2.13                     | 0.49              |
| 31:BJ:128:ASN:ND2  | 31:BJ:129:GLU:H    | 2.11                     | 0.49              |
| 35:BN:34:ILE:HD13  | 35:BN:34:ILE:H     | 1.76                     | 0.49              |
| 37:BP:23:ASP:O     | 37:BP:25:VAL:N     | 2.46                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 39:BR:47:VAL:C    | 39:BR:49:ILE:H     | 2.20                     | 0.49              |
| 39:BR:69:GLY:HA2  | 39:BR:96:VAL:HA    | 1.94                     | 0.49              |
| 43:BW:47:GLY:HA2  | 43:BW:67:LYS:HZ3   | 1.77                     | 0.49              |
| 45:BY:18:LYS:HD2  | 45:BY:53:MET:CE    | 2.42                     | 0.49              |
| 52:BI:17:ALA:O    | 52:BI:18:ASN:HB3   | 2.12                     | 0.49              |
| 1:CA:317:U:H2'    | 1:CA:318:G:C8      | 2.47                     | 0.49              |
| 1:CA:966:G:H2'    | 1:CA:967:C:C6      | 2.47                     | 0.49              |
| 1:CA:1320:C:H41   | 18:CS:36:ARG:CD    | 2.25                     | 0.49              |
| 1:CA:1324:A:H2'   | 1:CA:1325:C:C6     | 2.48                     | 0.49              |
| 2:CC:108:PRO:C    | 2:CC:110:LEU:H     | 2.21                     | 0.49              |
| 4:CE:85:LYS:HE3   | 4:CE:94:PHE:HB2    | 1.95                     | 0.49              |
| 5:CF:84:VAL:HG22  | 5:CF:85:ILE:N      | 2.28                     | 0.49              |
| 6:CG:144:ALA:C    | 6:CG:146:ALA:N     | 2.71                     | 0.49              |
| 9:CJ:35:GLN:HB3   | 9:CJ:78:GLU:CD     | 2.37                     | 0.49              |
| 10:CK:31:VAL:HG21 | 10:CK:66:ALA:CA    | 2.42                     | 0.49              |
| 16:CQ:46:HIS:CG   | 16:CQ:47:ASP:N     | 2.81                     | 0.49              |
| 23:DB:345:A:H1'   | 23:DB:346:A:H2     | 1.77                     | 0.49              |
| 23:DB:383:C:N4    | 23:DB:385:C:H2'    | 2.27                     | 0.49              |
| 23:DB:778:G:H5''  | 25:DC:48:ILE:HG21  | 1.95                     | 0.49              |
| 23:DB:845:A:C2    | 23:DB:847:U:H1'    | 2.47                     | 0.49              |
| 23:DB:1259:G:H2'  | 23:DB:1260:A:C8    | 2.48                     | 0.49              |
| 23:DB:1684:G:H2'  | 23:DB:1685:C:H6    | 1.77                     | 0.49              |
| 23:DB:2230:G:H5'' | 46:DZ:28:VAL:HG21  | 1.94                     | 0.49              |
| 23:DB:2734:A:C2'  | 23:DB:2735:G:H5'   | 2.43                     | 0.49              |
| 25:DC:163:ILE:O   | 25:DC:164:VAL:HG13 | 2.13                     | 0.49              |
| 25:DC:169:ALA:O   | 25:DC:170:TYR:HB2  | 2.13                     | 0.49              |
| 25:DC:231:HIS:CE1 | 25:DC:242:HIS:HD1  | 2.31                     | 0.49              |
| 26:DD:17:GLU:CG   | 37:DP:80:VAL:HB    | 2.42                     | 0.49              |
| 26:DD:205:PRO:HG2 | 26:DD:206:ALA:H    | 1.77                     | 0.49              |
| 27:DE:115:GLN:OE1 | 27:DE:184:ASP:HB2  | 2.13                     | 0.49              |
| 29:DG:79:THR:HG23 | 29:DG:80:GLU:H     | 1.78                     | 0.49              |
| 29:DG:163:TYR:C   | 29:DG:165:ASP:H    | 2.20                     | 0.49              |
| 31:DJ:7:LYS:HE3   | 31:DJ:47:HIS:HD2   | 1.76                     | 0.49              |
| 32:DK:63:VAL:HG11 | 32:DK:103:VAL:HG12 | 1.95                     | 0.49              |
| 37:DP:79:VAL:O    | 37:DP:81:ASP:N     | 2.46                     | 0.49              |
| 40:DS:2:GLU:CB    | 40:DS:108:SER:HA   | 2.41                     | 0.49              |
| 40:DS:29:VAL:HG21 | 40:DS:69:LEU:C     | 2.38                     | 0.49              |
| 42:DU:8:ASP:O     | 42:DU:10:VAL:HG13  | 2.13                     | 0.49              |
| 43:DW:10:ARG:HA   | 43:DW:10:ARG:HH11  | 1.77                     | 0.49              |
| 48:D1:7:LYS:HG2   | 48:D1:26:LYS:HB3   | 1.94                     | 0.49              |
| 52:DI:108:ILE:CG2 | 52:DI:128:ILE:HD13 | 2.43                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:157:U:O2'    | 1:AA:158:G:H5'     | 2.13                     | 0.49              |
| 1:AA:218:U:H2'    | 1:AA:219:U:H6      | 1.78                     | 0.49              |
| 1:AA:272:C:H2'    | 1:AA:273:U:C6      | 2.48                     | 0.49              |
| 1:AA:627:G:H2'    | 1:AA:628:G:H8      | 1.78                     | 0.49              |
| 1:AA:692:U:H2'    | 1:AA:694:A:OP2     | 2.13                     | 0.49              |
| 1:AA:846:G:H2'    | 1:AA:846:G:N3      | 2.27                     | 0.49              |
| 1:AA:975:A:H4'    | 1:AA:976:G:OP2     | 2.13                     | 0.49              |
| 4:AE:45:VAL:CG1   | 4:AE:116:VAL:HG23  | 2.43                     | 0.49              |
| 4:AE:45:VAL:HG13  | 4:AE:117:ALA:HA    | 1.95                     | 0.49              |
| 4:AE:67:ARG:O     | 4:AE:70:MET:HG3    | 2.13                     | 0.49              |
| 4:AE:104:ILE:HG23 | 4:AE:104:ILE:O     | 2.13                     | 0.49              |
| 5:AF:1:MET:SD     | 5:AF:67:PRO:HD3    | 2.53                     | 0.49              |
| 8:AI:24:ASN:HA    | 8:AI:26:LYS:HZ2    | 1.76                     | 0.49              |
| 8:AI:43:ALA:C     | 8:AI:45:MET:H      | 2.21                     | 0.49              |
| 9:AJ:53:ILE:HB    | 9:AJ:61:ALA:HB1    | 1.94                     | 0.49              |
| 16:AQ:10:ARG:NH1  | 16:AQ:11:VAL:HB    | 2.28                     | 0.49              |
| 16:AQ:20:ILE:CG1  | 16:AQ:45:VAL:HB    | 2.37                     | 0.49              |
| 16:AQ:60:ILE:HB   | 16:AQ:72:TRP:HE3   | 1.78                     | 0.49              |
| 20:AB:27:LYS:H    | 20:AB:28:PRO:CD    | 2.25                     | 0.49              |
| 20:AB:67:LEU:HA   | 20:AB:89:PHE:O     | 2.11                     | 0.49              |
| 20:AB:113:LEU:C   | 20:AB:113:LEU:HD23 | 2.37                     | 0.49              |
| 23:BB:354:A:C2'   | 23:BB:355:U:H5''   | 2.42                     | 0.49              |
| 23:BB:638:G:H2'   | 23:BB:639:U:C6     | 2.48                     | 0.49              |
| 23:BB:673:C:H5''  | 27:BE:76:PRO:HD2   | 1.94                     | 0.49              |
| 23:BB:1533:C:C2'  | 23:BB:1534:U:H5'   | 2.42                     | 0.49              |
| 23:BB:1568:G:C5'  | 25:BC:60:ALA:HB3   | 2.42                     | 0.49              |
| 23:BB:1581:G:O2'  | 23:BB:1582:C:H5'   | 2.13                     | 0.49              |
| 23:BB:1821:A:H2'  | 23:BB:1822:C:H6    | 1.76                     | 0.49              |
| 23:BB:2080:A:H2'  | 23:BB:2081:U:C6    | 2.48                     | 0.49              |
| 23:BB:2133:G:N3   | 23:BB:2133:G:C2'   | 2.73                     | 0.49              |
| 23:BB:2336:A:C1'  | 23:BB:2337:G:OP1   | 2.56                     | 0.49              |
| 23:BB:2500:U:H5'  | 23:BB:2501:C:OP2   | 2.12                     | 0.49              |
| 25:BC:70:LYS:HG2  | 25:BC:71:ASP:N     | 2.28                     | 0.49              |
| 26:BD:29:VAL:O    | 26:BD:51:THR:HG21  | 2.13                     | 0.49              |
| 26:BD:117:GLY:O   | 26:BD:165:MET:HB3  | 2.13                     | 0.49              |
| 27:BE:152:GLU:O   | 27:BE:153:LEU:HB2  | 2.12                     | 0.49              |
| 28:BF:2:LYS:HE2   | 28:BF:2:LYS:HA     | 1.92                     | 0.49              |
| 28:BF:165:GLY:O   | 28:BF:167:ALA:N    | 2.44                     | 0.49              |
| 28:BF:177:ARG:HE  | 28:BF:177:ARG:C    | 2.21                     | 0.49              |
| 31:BJ:118:MET:O   | 31:BJ:121:LYS:HB2  | 2.13                     | 0.49              |
| 39:BR:40:MET:CA   | 39:BR:54:VAL:HG11  | 2.43                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:BR:97:LYS:O    | 39:BR:98:ILE:HB   | 2.13                     | 0.49              |
| 43:BW:24:ARG:HA   | 43:BW:57:THR:HG23 | 1.93                     | 0.49              |
| 43:BW:37:VAL:O    | 43:BW:38:ARG:C    | 2.55                     | 0.49              |
| 50:B3:12:ARG:CB   | 50:B3:23:HIS:HA   | 2.34                     | 0.49              |
| 51:B4:23:ILE:HD12 | 51:B4:35:GLN:HG2  | 1.95                     | 0.49              |
| 52:BI:7:TYR:C     | 52:BI:7:TYR:CD1   | 2.91                     | 0.49              |
| 1:CA:376:G:C4'    | 15:CP:5:ARG:HD3   | 2.42                     | 0.49              |
| 1:CA:708:C:H2'    | 1:CA:709:U:C6     | 2.48                     | 0.49              |
| 1:CA:1014:A:H2    | 1:CA:1219:A:H1'   | 1.76                     | 0.49              |
| 1:CA:1281:C:H5'   | 1:CA:1282:C:C5    | 2.43                     | 0.49              |
| 1:CA:1312:G:H2'   | 1:CA:1313:U:C6    | 2.48                     | 0.49              |
| 1:CA:1366:C:H2'   | 1:CA:1367:C:C6    | 2.47                     | 0.49              |
| 1:CA:1522:U:O2'   | 1:CA:1523:G:H5'   | 2.13                     | 0.49              |
| 7:CH:38:VAL:HG23  | 7:CH:111:THR:HG22 | 1.94                     | 0.49              |
| 10:CK:18:GLY:HA2  | 10:CK:35:ASP:HA   | 1.95                     | 0.49              |
| 15:CP:54:LEU:HD22 | 15:CP:80:LYS:HZ2  | 1.77                     | 0.49              |
| 16:CQ:12:VAL:HG11 | 16:CQ:42:LYS:NZ   | 2.27                     | 0.49              |
| 18:CS:62:THR:HG22 | 18:CS:65:MET:CE   | 2.43                     | 0.49              |
| 19:CT:68:LYS:HE2  | 19:CT:68:LYS:CA   | 2.37                     | 0.49              |
| 20:CB:14:HIS:CG   | 20:CB:15:PHE:N    | 2.80                     | 0.49              |
| 20:CB:26:MET:HG3  | 20:CB:188:THR:O   | 2.13                     | 0.49              |
| 23:DB:281:C:H2'   | 23:DB:281:C:O2    | 2.11                     | 0.49              |
| 23:DB:1266:G:OP1  | 47:D0:15:ARG:NH2  | 2.45                     | 0.49              |
| 23:DB:1315:C:H2'  | 23:DB:1316:U:H6   | 1.77                     | 0.49              |
| 23:DB:1383:A:H2   | 23:DB:1405:U:O2   | 1.96                     | 0.49              |
| 23:DB:1904:G:H1'  | 23:DB:1927:A:N1   | 2.28                     | 0.49              |
| 23:DB:2034:U:H5'' | 55:DB:3318:HOH:O  | 2.13                     | 0.49              |
| 23:DB:2278:A:H62  | 43:DW:10:ARG:CB   | 2.26                     | 0.49              |
| 23:DB:2468:A:H2'  | 23:DB:2476:A:C6   | 2.48                     | 0.49              |
| 23:DB:2740:A:H2'  | 23:DB:2741:A:C8   | 2.47                     | 0.49              |
| 23:DB:2896:C:H2'  | 23:DB:2897:U:C6   | 2.47                     | 0.49              |
| 26:DD:4:LEU:HD11  | 26:DD:79:LEU:HD22 | 1.93                     | 0.49              |
| 29:DG:156:TYR:HA  | 29:DG:171:LYS:CG  | 2.43                     | 0.49              |
| 31:DJ:64:VAL:CG1  | 31:DJ:65:THR:H    | 2.19                     | 0.49              |
| 32:DK:70:ARG:HD3  | 32:DK:76:VAL:CG2  | 2.36                     | 0.49              |
| 33:DL:61:LEU:HD23 | 33:DL:61:LEU:C    | 2.38                     | 0.49              |
| 39:DR:68:ARG:HB3  | 39:DR:70:GLU:HG2  | 1.93                     | 0.49              |
| 43:DW:4:LYS:HZ3   | 43:DW:4:LYS:HB2   | 1.78                     | 0.49              |
| 45:DY:2:LYS:CE    | 45:DY:27:GLY:H    | 2.26                     | 0.49              |
| 46:DZ:25:ARG:O    | 46:DZ:26:SER:HB3  | 2.11                     | 0.49              |
| 51:D4:1:MET:HE3   | 51:D4:2:LYS:CD    | 2.43                     | 0.49              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:16:A:H4'      | 4:AE:21:SER:H      | 1.77                     | 0.49              |
| 1:AA:176:C:H2'     | 1:AA:177:G:N3      | 2.26                     | 0.49              |
| 1:AA:626:G:H2'     | 1:AA:627:G:C8      | 2.48                     | 0.49              |
| 1:AA:1103:C:C5'    | 20:AB:96:LEU:HD12  | 2.42                     | 0.49              |
| 1:AA:1121:U:O2'    | 1:AA:1122:U:H5'    | 2.13                     | 0.49              |
| 1:AA:1371:G:OP1    | 8:AI:12:LYS:HG2    | 2.12                     | 0.49              |
| 2:AC:61:LYS:O      | 2:AC:97:PRO:HD2    | 2.13                     | 0.49              |
| 9:AJ:41:PRO:O      | 9:AJ:42:LEU:HB2    | 2.13                     | 0.49              |
| 15:AP:43:ALA:O     | 15:AP:46:LYS:HD3   | 2.12                     | 0.49              |
| 20:AB:162:VAL:HG21 | 20:AB:168:GLU:HB2  | 1.94                     | 0.49              |
| 22:BA:82:U:O2'     | 22:BA:83:G:H5'     | 2.13                     | 0.49              |
| 23:BB:154:U:H2'    | 23:BB:155:A:C8     | 2.48                     | 0.49              |
| 23:BB:967:U:H2'    | 23:BB:968:C:H6     | 1.73                     | 0.49              |
| 23:BB:1206:G:H2'   | 23:BB:1207:C:H6    | 1.78                     | 0.49              |
| 23:BB:1268:A:H2'   | 23:BB:1269:A:O4'   | 2.13                     | 0.49              |
| 23:BB:1904:G:H1'   | 23:BB:1927:A:N1    | 2.28                     | 0.49              |
| 23:BB:2390:U:O2'   | 23:BB:2391:G:H5''  | 2.12                     | 0.49              |
| 23:BB:2488:G:O2'   | 23:BB:2489:U:H5'   | 2.12                     | 0.49              |
| 23:BB:2563:U:H2'   | 23:BB:2565:A:OP2   | 2.13                     | 0.49              |
| 23:BB:2896:C:H2'   | 23:BB:2897:U:H6    | 1.78                     | 0.49              |
| 25:BC:212:TRP:CZ3  | 25:BC:217:PRO:HD3  | 2.48                     | 0.49              |
| 27:BE:29:HIS:O     | 27:BE:33:VAL:HG23  | 2.12                     | 0.49              |
| 27:BE:111:GLU:C    | 27:BE:113:VAL:H    | 2.21                     | 0.49              |
| 28:BF:55:ASP:OD1   | 28:BF:148:VAL:HG11 | 2.13                     | 0.49              |
| 32:BK:54:LYS:HD3   | 32:BK:54:LYS:N     | 2.28                     | 0.49              |
| 34:BM:71:LYS:HD3   | 34:BM:92:TRP:O     | 2.12                     | 0.49              |
| 34:BM:130:PHE:HD2  | 34:BM:131:VAL:HG22 | 1.77                     | 0.49              |
| 35:BN:2:ARG:O      | 35:BN:3:HIS:CG     | 2.66                     | 0.49              |
| 35:BN:13:ASN:O     | 35:BN:17:ARG:N     | 2.44                     | 0.49              |
| 35:BN:57:THR:OG1   | 35:BN:61:ALA:HB3   | 2.12                     | 0.49              |
| 37:BP:92:ARG:HH22  | 37:BP:110:LYS:HE2  | 1.75                     | 0.49              |
| 42:BU:90:LYS:NZ    | 42:BU:91:LYS:HE2   | 2.23                     | 0.49              |
| 44:BX:8:GLU:O      | 44:BX:10:SER:N     | 2.46                     | 0.49              |
| 1:CA:193:C:H2'     | 1:CA:194:C:C6      | 2.47                     | 0.49              |
| 1:CA:382:A:H2'     | 1:CA:383:A:C8      | 2.48                     | 0.49              |
| 1:CA:1308:U:P      | 12:CM:97:ARG:HD3   | 2.53                     | 0.49              |
| 4:CE:99:SER:C      | 4:CE:101:GLY:H     | 2.20                     | 0.49              |
| 6:CG:8:GLN:NE2     | 6:CG:9:ARG:H       | 2.10                     | 0.49              |
| 9:CJ:46:LYS:HA     | 9:CJ:68:ARG:HA     | 1.95                     | 0.49              |
| 9:CJ:67:ILE:O      | 9:CJ:67:ILE:HG23   | 2.13                     | 0.49              |
| 10:CK:69:CYS:O     | 10:CK:73:VAL:HG13  | 2.12                     | 0.49              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:CK:110:THR:CG2 | 21:CU:4:LYS:HA    | 2.43                     | 0.49              |
| 16:CQ:68:LYS:C    | 16:CQ:70:LYS:N    | 2.70                     | 0.49              |
| 17:CR:42:ARG:C    | 17:CR:44:THR:H    | 2.21                     | 0.49              |
| 18:CS:5:LYS:C     | 18:CS:6:LYS:HG2   | 2.38                     | 0.49              |
| 19:CT:66:ILE:HG13 | 19:CT:70:LYS:HG3  | 1.95                     | 0.49              |
| 23:DB:170:U:H2'   | 23:DB:171:U:H6    | 1.78                     | 0.49              |
| 23:DB:208:C:H2'   | 23:DB:209:C:C6    | 2.47                     | 0.49              |
| 23:DB:242:G:O2'   | 23:DB:243:U:P     | 2.70                     | 0.49              |
| 23:DB:312:G:H2'   | 23:DB:313:G:H8    | 1.78                     | 0.49              |
| 23:DB:318:C:O2'   | 23:DB:319:G:H5'   | 2.12                     | 0.49              |
| 23:DB:346:A:C8    | 23:DB:347:A:H1'   | 2.48                     | 0.49              |
| 23:DB:367:G:H2'   | 23:DB:368:A:O4'   | 2.12                     | 0.49              |
| 23:DB:452:G:N2    | 23:DB:457:A:O2'   | 2.46                     | 0.49              |
| 23:DB:638:G:H2'   | 23:DB:639:U:C6    | 2.48                     | 0.49              |
| 23:DB:1083:U:C2   | 23:DB:1086:A:N1   | 2.81                     | 0.49              |
| 23:DB:1112:G:H4'  | 29:DG:1:SER:O     | 2.13                     | 0.49              |
| 23:DB:1142:A:C4   | 23:DB:1144:A:C8   | 3.01                     | 0.49              |
| 23:DB:1463:C:H2'  | 23:DB:1464:G:C8   | 2.48                     | 0.49              |
| 23:DB:2484:G:N2   | 34:DM:118:LYS:HG2 | 2.27                     | 0.49              |
| 23:DB:2809:A:H2'  | 23:DB:2810:A:H8   | 1.77                     | 0.49              |
| 23:DB:2869:G:H2'  | 23:DB:2870:C:H6   | 1.75                     | 0.49              |
| 26:DD:18:ASP:C    | 26:DD:20:VAL:N    | 2.70                     | 0.49              |
| 28:DF:41:GLU:O    | 28:DF:43:ILE:N    | 2.46                     | 0.49              |
| 31:DJ:54:ILE:HG22 | 31:DJ:55:ILE:N    | 2.27                     | 0.49              |
| 31:DJ:122:LEU:O   | 31:DJ:123:LYS:HB2 | 2.11                     | 0.49              |
| 36:DO:58:ILE:HG13 | 36:DO:60:GLU:H    | 1.77                     | 0.49              |
| 39:DR:67:GLY:H    | 39:DR:98:ILE:CA   | 2.26                     | 0.49              |
| 40:DS:3:THR:O     | 40:DS:4:ILE:HB    | 2.13                     | 0.49              |
| 44:DX:15:ASN:HA   | 44:DX:17:GLU:OE2  | 2.13                     | 0.49              |
| 46:DZ:2:LYS:O     | 46:DZ:3:LYS:C     | 2.55                     | 0.49              |
| 47:D0:36:LYS:HG3  | 47:D0:40:HIS:C    | 2.38                     | 0.49              |
| 1:AA:22:G:H2'     | 1:AA:23:C:C6      | 2.47                     | 0.49              |
| 1:AA:471:U:H2'    | 1:AA:472:U:C6     | 2.47                     | 0.49              |
| 1:AA:627:G:H2'    | 1:AA:628:G:C8     | 2.48                     | 0.49              |
| 1:AA:1343:G:H1'   | 8:AI:122:ARG:HH12 | 1.78                     | 0.49              |
| 2:AC:190:THR:HG22 | 2:AC:191:THR:H    | 1.78                     | 0.49              |
| 3:AD:150:LYS:HB2  | 3:AD:150:LYS:HZ3  | 1.78                     | 0.49              |
| 5:AF:54:LEU:HD13  | 5:AF:55:HIS:N     | 2.27                     | 0.49              |
| 6:AG:139:ASP:HA   | 6:AG:142:ARG:NH1  | 2.28                     | 0.49              |
| 7:AH:73:SER:HB2   | 7:AH:129:ALA:HB3  | 1.94                     | 0.49              |
| 11:AL:54:VAL:HG12 | 11:AL:56:LEU:HD12 | 1.95                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 13:AN:74:ARG:HG3  | 13:AN:74:ARG:HH11  | 1.77                     | 0.49              |
| 22:BA:113:C:H2'   | 22:BA:114:C:C6     | 2.48                     | 0.49              |
| 23:BB:336:C:O2'   | 23:BB:337:C:H5'    | 2.12                     | 0.49              |
| 23:BB:443:A:H2    | 23:BB:1245:G:N3    | 2.11                     | 0.49              |
| 23:BB:583:G:OP1   | 38:BQ:6:GLY:HA2    | 2.13                     | 0.49              |
| 23:BB:678:C:H2'   | 23:BB:679:C:H6     | 1.77                     | 0.49              |
| 23:BB:875:G:H2'   | 23:BB:876:C:O2     | 2.12                     | 0.49              |
| 23:BB:910:A:H2'   | 23:BB:911:A:C8     | 2.47                     | 0.49              |
| 23:BB:969:G:N2    | 23:BB:985:C:OP1    | 2.41                     | 0.49              |
| 23:BB:1120:G:O2'  | 23:BB:1121:C:H5'   | 2.13                     | 0.49              |
| 23:BB:1383:A:H2   | 23:BB:1405:U:O2    | 1.95                     | 0.49              |
| 23:BB:2354:C:H4'  | 43:BW:30:VAL:CG2   | 2.38                     | 0.49              |
| 23:BB:2372:U:OP1  | 48:B1:44:GLN:HG3   | 2.13                     | 0.49              |
| 23:BB:2803:G:H2'  | 23:BB:2804:U:C6    | 2.47                     | 0.49              |
| 25:BC:68:ARG:CD   | 25:BC:127:ASN:HD21 | 2.26                     | 0.49              |
| 26:BD:51:THR:O    | 26:BD:52:THR:HB    | 2.13                     | 0.49              |
| 26:BD:92:VAL:HG13 | 26:BD:94:GLN:H     | 1.78                     | 0.49              |
| 27:BE:108:ILE:H   | 27:BE:108:ILE:CD1  | 2.26                     | 0.49              |
| 27:BE:127:GLU:O   | 27:BE:157:LEU:HD22 | 2.13                     | 0.49              |
| 28:BF:172:PHE:CD1 | 28:BF:173:ASP:N    | 2.80                     | 0.49              |
| 30:BH:23:ALA:C    | 30:BH:25:TYR:H     | 2.21                     | 0.49              |
| 30:BH:29:PHE:CD2  | 30:BH:30:LEU:HD23  | 2.48                     | 0.49              |
| 34:BM:62:LYS:HB3  | 34:BM:104:GLU:HB2  | 1.95                     | 0.49              |
| 35:BN:52:ILE:HG21 | 35:BN:94:TYR:CE2   | 2.48                     | 0.49              |
| 35:BN:65:LEU:CD1  | 35:BN:68:ALA:HB3   | 2.43                     | 0.49              |
| 36:BO:8:ILE:HG22  | 36:BO:10:ARG:H     | 1.77                     | 0.49              |
| 37:BP:16:VAL:N    | 37:BP:17:PRO:HD3   | 2.28                     | 0.49              |
| 37:BP:18:SER:C    | 37:BP:20:ARG:H     | 2.21                     | 0.49              |
| 38:BQ:102:LYS:HG2 | 38:BQ:103:VAL:H    | 1.77                     | 0.49              |
| 43:BW:47:GLY:N    | 43:BW:67:LYS:NZ    | 2.60                     | 0.49              |
| 46:BZ:61:ASN:O    | 46:BZ:65:ASN:N     | 2.46                     | 0.49              |
| 49:B2:34:ARG:HH11 | 49:B2:34:ARG:HG3   | 1.77                     | 0.49              |
| 52:BI:63:ASP:C    | 52:BI:65:SER:N     | 2.67                     | 0.49              |
| 52:BI:109:ALA:HB1 | 52:BI:124:MET:CG   | 2.42                     | 0.49              |
| 1:CA:35:G:H2'     | 1:CA:36:C:H6       | 1.78                     | 0.49              |
| 1:CA:71:A:O2'     | 1:CA:72:A:H5''     | 2.13                     | 0.49              |
| 1:CA:84:U:O2'     | 1:CA:86:G:N2       | 2.46                     | 0.49              |
| 1:CA:301:G:H2'    | 1:CA:302:G:C8      | 2.48                     | 0.49              |
| 1:CA:975:A:H61    | 9:CJ:50:THR:HB     | 1.77                     | 0.49              |
| 1:CA:1031:C:H5'   | 1:CA:1032:G:C8     | 2.48                     | 0.49              |
| 1:CA:1231:G:O2'   | 1:CA:1232:U:H5'    | 2.13                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1243:C:H2'   | 1:CA:1244:G:H8    | 1.78                     | 0.49              |
| 1:CA:1356:G:H2'   | 1:CA:1357:A:C8    | 2.48                     | 0.49              |
| 2:CC:2:GLN:H      | 2:CC:2:GLN:NE2    | 2.10                     | 0.49              |
| 3:CD:138:PRO:O    | 3:CD:139:ASN:HB3  | 2.12                     | 0.49              |
| 9:CJ:8:ILE:O      | 9:CJ:8:ILE:HG13   | 2.13                     | 0.49              |
| 9:CJ:15:HIS:HA    | 9:CJ:18:ILE:HG22  | 1.94                     | 0.49              |
| 10:CK:70:ALA:C    | 10:CK:72:ALA:N    | 2.70                     | 0.49              |
| 12:CM:63:VAL:HG12 | 12:CM:68:LEU:HB2  | 1.95                     | 0.49              |
| 14:CO:25:GLU:CD   | 14:CO:76:ARG:HD3  | 2.38                     | 0.49              |
| 15:CP:3:THR:CG2   | 15:CP:66:THR:HB   | 2.39                     | 0.49              |
| 15:CP:20:VAL:HG21 | 15:CP:32:PHE:CD2  | 2.48                     | 0.49              |
| 16:CQ:30:HIS:CE1  | 16:CQ:32:ILE:HG22 | 2.48                     | 0.49              |
| 16:CQ:43:LEU:HD12 | 16:CQ:43:LEU:N    | 2.27                     | 0.49              |
| 22:DA:109:A:H2'   | 22:DA:110:C:C6    | 2.48                     | 0.49              |
| 23:DB:485:C:O2'   | 23:DB:486:C:H5'   | 2.12                     | 0.49              |
| 23:DB:518:G:H2'   | 23:DB:519:U:C6    | 2.48                     | 0.49              |
| 23:DB:1439:A:C8   | 23:DB:1440:U:C6   | 3.01                     | 0.49              |
| 23:DB:1847:A:H4'  | 23:DB:1848:A:H8   | 1.78                     | 0.49              |
| 23:DB:2737:G:H2'  | 23:DB:2738:A:C8   | 2.48                     | 0.49              |
| 23:DB:2893:A:H4'  | 23:DB:2894:G:C5'  | 2.43                     | 0.49              |
| 25:DC:12:ARG:HG3  | 25:DC:19:VAL:O    | 2.13                     | 0.49              |
| 27:DE:48:THR:HG23 | 27:DE:85:PHE:H    | 1.78                     | 0.49              |
| 27:DE:138:LEU:HB2 | 27:DE:143:LEU:HG  | 1.94                     | 0.49              |
| 28:DF:8:LYS:HA    | 28:DF:12:VAL:HG23 | 1.94                     | 0.49              |
| 29:DG:29:ASN:CB   | 29:DG:78:VAL:HA   | 2.42                     | 0.49              |
| 30:DH:3:VAL:HG21  | 30:DH:37:VAL:HG21 | 1.95                     | 0.49              |
| 32:DK:104:THR:HB  | 32:DK:106:GLU:OE1 | 2.13                     | 0.49              |
| 33:DL:75:ALA:HB3  | 33:DL:108:ALA:HA  | 1.94                     | 0.49              |
| 40:DS:43:ALA:C    | 40:DS:45:VAL:H    | 2.20                     | 0.49              |
| 42:DU:11:ILE:HG22 | 42:DU:19:GLY:HA2  | 1.94                     | 0.49              |
| 42:DU:28:LEU:HD11 | 42:DU:31:GLY:CA   | 2.43                     | 0.49              |
| 44:DX:22:LEU:HD22 | 44:DX:25:GLN:CD   | 2.38                     | 0.49              |
| 50:D3:4:LYS:CE    | 50:D3:61:LEU:H    | 2.26                     | 0.49              |
| 1:AA:448:A:O2'    | 1:AA:449:G:H5'    | 2.13                     | 0.48              |
| 1:AA:600:A:H2'    | 1:AA:601:G:C8     | 2.48                     | 0.48              |
| 1:AA:920:U:H2'    | 1:AA:921:U:C6     | 2.48                     | 0.48              |
| 1:AA:970:C:C5     | 1:AA:1231:G:H1'   | 2.48                     | 0.48              |
| 1:AA:1126:U:O2'   | 1:AA:1280:A:H2'   | 2.13                     | 0.48              |
| 1:AA:1172:C:H2'   | 1:AA:1173:U:C6    | 2.48                     | 0.48              |
| 3:AD:107:GLY:HA2  | 3:AD:112:GLU:OE1  | 2.13                     | 0.48              |
| 4:AE:33:THR:O     | 4:AE:34:ALA:CB    | 2.61                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:AI:30:ASN:ND2   | 8:AI:30:ASN:N      | 2.59                     | 0.48              |
| 8:AI:90:ASP:O     | 8:AI:93:LEU:HG     | 2.13                     | 0.48              |
| 23:BB:91:A:H2'    | 23:BB:92:U:C6      | 2.48                     | 0.48              |
| 23:BB:100:U:C4'   | 42:BU:90:LYS:HE2   | 2.26                     | 0.48              |
| 23:BB:435:C:H2'   | 23:BB:436:C:H5'    | 1.94                     | 0.48              |
| 23:BB:866:A:H61   | 23:BB:913:U:H4'    | 1.78                     | 0.48              |
| 23:BB:904:G:H2'   | 23:BB:905:A:H8     | 1.78                     | 0.48              |
| 23:BB:929:U:H2'   | 23:BB:930:G:C8     | 2.47                     | 0.48              |
| 23:BB:1544:A:H2'  | 23:BB:1545:A:C8    | 2.48                     | 0.48              |
| 23:BB:1594:U:H2'  | 23:BB:1595:C:H6    | 1.75                     | 0.48              |
| 23:BB:1601:G:OP1  | 41:BT:62:VAL:HG21  | 2.14                     | 0.48              |
| 23:BB:1747:U:H2'  | 23:BB:1748:C:C6    | 2.47                     | 0.48              |
| 23:BB:2335:A:P    | 36:BO:9:ARG:HG3    | 2.53                     | 0.48              |
| 23:BB:2834:G:H2'  | 23:BB:2879:A:N6    | 2.28                     | 0.48              |
| 28:BF:18:GLU:HA   | 28:BF:18:GLU:OE2   | 2.12                     | 0.48              |
| 28:BF:135:ILE:O   | 28:BF:137:PHE:N    | 2.46                     | 0.48              |
| 29:BG:84:LYS:HA   | 29:BG:84:LYS:NZ    | 2.28                     | 0.48              |
| 33:BL:85:VAL:HG22 | 33:BL:98:ALA:HB2   | 1.94                     | 0.48              |
| 34:BM:58:LYS:C    | 34:BM:60:GLN:N     | 2.71                     | 0.48              |
| 36:BO:8:ILE:HG22  | 36:BO:10:ARG:CG    | 2.38                     | 0.48              |
| 36:BO:62:LEU:O    | 36:BO:64:TYR:N     | 2.45                     | 0.48              |
| 37:BP:23:ASP:H    | 37:BP:93:LYS:HZ1   | 1.60                     | 0.48              |
| 37:BP:48:ALA:C    | 37:BP:49:ILE:HG13  | 2.38                     | 0.48              |
| 39:BR:33:VAL:HB   | 39:BR:35:PHE:CE2   | 2.48                     | 0.48              |
| 42:BU:46:LYS:N    | 42:BU:47:PRO:CD    | 2.72                     | 0.48              |
| 42:BU:99:SER:OG   | 42:BU:102:ILE:HD11 | 2.13                     | 0.48              |
| 1:CA:471:U:H2'    | 1:CA:472:U:C6      | 2.47                     | 0.48              |
| 1:CA:916:U:H2'    | 1:CA:917:G:H8      | 1.78                     | 0.48              |
| 1:CA:1004:A:H2'   | 1:CA:1005:A:O4'    | 2.13                     | 0.48              |
| 1:CA:1275:A:H2'   | 1:CA:1276:G:C8     | 2.47                     | 0.48              |
| 4:CE:17:VAL:O     | 4:CE:17:VAL:HG13   | 2.12                     | 0.48              |
| 5:CF:18:VAL:N     | 5:CF:19:PRO:HD2    | 2.27                     | 0.48              |
| 5:CF:100:SER:H    | 17:CR:23:LYS:NZ    | 2.11                     | 0.48              |
| 6:CG:64:ALA:O     | 6:CG:67:ASN:HB2    | 2.13                     | 0.48              |
| 8:CI:22:PRO:HA    | 8:CI:60:LEU:HA     | 1.94                     | 0.48              |
| 11:CL:17:LYS:HB2  | 11:CL:17:LYS:HZ2   | 1.75                     | 0.48              |
| 12:CM:102:LYS:HG3 | 12:CM:103:THR:H    | 1.77                     | 0.48              |
| 16:CQ:30:HIS:CG   | 16:CQ:33:TYR:HB2   | 2.48                     | 0.48              |
| 20:CB:218:ALA:CA  | 20:CB:221:ARG:HG2  | 2.41                     | 0.48              |
| 23:DB:39:G:H2'    | 23:DB:40:U:C6      | 2.48                     | 0.48              |
| 23:DB:353:C:O2    | 23:DB:353:C:H2'    | 2.13                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:372:G:C8     | 46:DZ:57:VAL:HG21  | 2.48                     | 0.48              |
| 23:DB:409:G:H2'    | 23:DB:410:G:C8     | 2.48                     | 0.48              |
| 23:DB:543:G:H2'    | 23:DB:545:U:OP1    | 2.13                     | 0.48              |
| 23:DB:685:A:H1'    | 23:DB:688:U:O4     | 2.13                     | 0.48              |
| 23:DB:833:A:H2'    | 23:DB:834:G:H8     | 1.73                     | 0.48              |
| 23:DB:899:A:C2     | 23:DB:900:A:H1'    | 2.48                     | 0.48              |
| 23:DB:1051:G:H2'   | 23:DB:1052:C:C6    | 2.47                     | 0.48              |
| 23:DB:1153:C:O2'   | 23:DB:1154:G:H5'   | 2.13                     | 0.48              |
| 23:DB:1412:U:H2'   | 23:DB:1413:A:H8    | 1.76                     | 0.48              |
| 23:DB:1583:A:H4'   | 23:DB:1585:C:N3    | 2.29                     | 0.48              |
| 23:DB:1814:G:H5'   | 25:DC:51:ARG:HG2   | 1.95                     | 0.48              |
| 23:DB:2390:U:O2'   | 23:DB:2391:G:H5''  | 2.12                     | 0.48              |
| 23:DB:2812:G:H2'   | 23:DB:2813:A:O4'   | 2.13                     | 0.48              |
| 25:DC:171:VAL:HG23 | 25:DC:182:LYS:NZ   | 2.27                     | 0.48              |
| 26:DD:27:ILE:HD13  | 26:DD:27:ILE:C     | 2.37                     | 0.48              |
| 26:DD:34:VAL:HG12  | 26:DD:91:THR:HG22  | 1.94                     | 0.48              |
| 26:DD:81:GLU:O     | 26:DD:82:PHE:HB2   | 2.13                     | 0.48              |
| 26:DD:202:ILE:CG2  | 26:DD:204:LYS:HG2  | 2.42                     | 0.48              |
| 27:DE:24:ASN:N     | 27:DE:110:SER:HB2  | 2.27                     | 0.48              |
| 28:DF:39:VAL:CG2   | 28:DF:84:ILE:HD13  | 2.42                     | 0.48              |
| 28:DF:83:PRO:HG2   | 28:DF:84:ILE:H     | 1.78                     | 0.48              |
| 29:DG:67:ALA:O     | 29:DG:71:LEU:HG    | 2.12                     | 0.48              |
| 32:DK:66:LYS:HE3   | 32:DK:80:ASP:O     | 2.12                     | 0.48              |
| 33:DL:125:LEU:O    | 33:DL:127:VAL:HG13 | 2.13                     | 0.48              |
| 34:DM:6:ARG:CD     | 34:DM:71:LYS:HE3   | 2.42                     | 0.48              |
| 37:DP:50:ARG:CG    | 37:DP:99:LEU:H     | 2.25                     | 0.48              |
| 38:DQ:82:LEU:HG    | 38:DQ:88:GLU:HG3   | 1.93                     | 0.48              |
| 38:DQ:88:GLU:O     | 38:DQ:89:ILE:C     | 2.56                     | 0.48              |
| 40:DS:27:LYS:N     | 40:DS:70:LYS:O     | 2.46                     | 0.48              |
| 43:DW:69:GLU:HG3   | 43:DW:70:VAL:N     | 2.24                     | 0.48              |
| 44:DX:18:LEU:HA    | 44:DX:22:LEU:CD1   | 2.37                     | 0.48              |
| 44:DX:18:LEU:HD12  | 44:DX:47:ARG:NH2   | 2.28                     | 0.48              |
| 46:DZ:25:ARG:HG3   | 46:DZ:26:SER:N     | 2.28                     | 0.48              |
| 52:DI:54:ILE:HD13  | 52:DI:54:ILE:C     | 2.37                     | 0.48              |
| 1:AA:140:U:H2'     | 1:AA:141:G:C8      | 2.48                     | 0.48              |
| 1:AA:236:A:H2'     | 1:AA:237:G:H8      | 1.78                     | 0.48              |
| 1:AA:405:U:OP2     | 3:AD:114:ARG:NH2   | 2.47                     | 0.48              |
| 1:AA:546:A:P       | 3:AD:68:GLU:HB3    | 2.53                     | 0.48              |
| 1:AA:560:A:H4'     | 1:AA:561:U:H5''    | 1.94                     | 0.48              |
| 1:AA:766:A:C2      | 1:AA:1525:G:N3     | 2.81                     | 0.48              |
| 1:AA:797:C:OP1     | 10:AK:125:LYS:HG2  | 2.13                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:806:C:H2'    | 1:AA:807:A:C8     | 2.47                     | 0.48              |
| 1:AA:893:C:H2'    | 1:AA:894:G:H8     | 1.78                     | 0.48              |
| 1:AA:901:A:H5'    | 1:AA:902:G:OP2    | 2.13                     | 0.48              |
| 1:AA:940:C:H2'    | 1:AA:941:G:C8     | 2.48                     | 0.48              |
| 1:AA:1314:C:H2'   | 1:AA:1315:U:H6    | 1.77                     | 0.48              |
| 1:AA:1510:C:H2'   | 1:AA:1511:G:H8    | 1.78                     | 0.48              |
| 4:AE:19:ARG:O     | 4:AE:20:VAL:HB    | 2.12                     | 0.48              |
| 4:AE:90:GLY:O     | 4:AE:128:GLY:HA3  | 2.13                     | 0.48              |
| 8:AI:9:GLY:HA2    | 8:AI:80:HIS:CD2   | 2.48                     | 0.48              |
| 9:AJ:88:MET:H     | 9:AJ:88:MET:CE    | 2.25                     | 0.48              |
| 10:AK:57:SER:O    | 10:AK:90:PRO:HG2  | 2.13                     | 0.48              |
| 11:AL:49:ARG:C    | 11:AL:50:LYS:HE2  | 2.38                     | 0.48              |
| 12:AM:56:ARG:O    | 12:AM:59:VAL:HG12 | 2.13                     | 0.48              |
| 17:AR:63:TYR:C    | 17:AR:65:SER:H    | 2.21                     | 0.48              |
| 23:BB:82:U:H2'    | 23:BB:83:A:C8     | 2.48                     | 0.48              |
| 23:BB:523:C:H2'   | 23:BB:524:G:H8    | 1.78                     | 0.48              |
| 23:BB:587:C:H4'   | 23:BB:588:U:C6    | 2.48                     | 0.48              |
| 23:BB:956:G:H1'   | 34:BM:81:ARG:HH22 | 1.77                     | 0.48              |
| 23:BB:966:G:H2'   | 23:BB:967:U:C6    | 2.47                     | 0.48              |
| 23:BB:1032:A:OP1  | 51:B4:8:LYS:HB3   | 2.13                     | 0.48              |
| 23:BB:1040:A:H2   | 23:BB:1115:G:H22  | 1.59                     | 0.48              |
| 23:BB:1137:G:H2'  | 23:BB:1138:G:O4'  | 2.13                     | 0.48              |
| 23:BB:1287:A:H3'  | 23:BB:1288:G:N2   | 2.28                     | 0.48              |
| 23:BB:2734:A:C2'  | 23:BB:2735:G:H5'  | 2.43                     | 0.48              |
| 23:BB:2834:G:H2'  | 23:BB:2879:A:H61  | 1.78                     | 0.48              |
| 23:BB:2860:A:H2'  | 23:BB:2861:U:O4'  | 2.13                     | 0.48              |
| 23:BB:2868:A:H2'  | 23:BB:2869:G:H8   | 1.78                     | 0.48              |
| 25:BC:124:LYS:HZ3 | 25:BC:125:PRO:HD2 | 1.78                     | 0.48              |
| 26:BD:114:LYS:HB3 | 35:BN:3:HIS:HE1   | 1.77                     | 0.48              |
| 26:BD:135:GLY:C   | 26:BD:137:SER:H   | 2.21                     | 0.48              |
| 27:BE:128:ALA:HA  | 27:BE:157:LEU:CD2 | 2.42                     | 0.48              |
| 36:BO:8:ILE:CG2   | 36:BO:9:ARG:N     | 2.75                     | 0.48              |
| 37:BP:29:VAL:N    | 37:BP:44:GLY:HA3  | 2.29                     | 0.48              |
| 37:BP:112:ARG:NH1 | 37:BP:112:ARG:H   | 2.11                     | 0.48              |
| 39:BR:16:GLU:O    | 39:BR:18:GLN:N    | 2.45                     | 0.48              |
| 44:BX:14:LEU:HD11 | 44:BX:57:LEU:HD22 | 1.95                     | 0.48              |
| 46:BZ:3:LYS:HG2   | 46:BZ:8:LYS:HA    | 1.95                     | 0.48              |
| 46:BZ:15:SER:HB3  | 46:BZ:23:LYS:CD   | 2.43                     | 0.48              |
| 47:B0:35:GLU:C    | 47:B0:37:HIS:H    | 2.21                     | 0.48              |
| 48:B1:5:ARG:O     | 48:B1:27:ARG:HB2  | 2.14                     | 0.48              |
| 1:CA:1053:G:O2'   | 1:CA:1199:U:H5    | 1.96                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:CJ:41:PRO:O     | 9:CJ:42:LEU:HB2    | 2.12                     | 0.48              |
| 14:CO:88:ARG:HG3  | 14:CO:88:ARG:NH1   | 2.28                     | 0.48              |
| 16:CQ:10:ARG:CZ   | 16:CQ:11:VAL:N     | 2.76                     | 0.48              |
| 18:CS:3:SER:O     | 18:CS:4:LEU:HD12   | 2.12                     | 0.48              |
| 19:CT:73:ARG:O    | 19:CT:74:HIS:C     | 2.55                     | 0.48              |
| 23:DB:46:G:H2'    | 23:DB:47:C:C6      | 2.48                     | 0.48              |
| 23:DB:150:U:H2'   | 23:DB:151:C:C6     | 2.48                     | 0.48              |
| 23:DB:524:G:H5'   | 23:DB:539:G:N2     | 2.27                     | 0.48              |
| 23:DB:907:G:O2'   | 23:DB:908:C:H5'    | 2.12                     | 0.48              |
| 23:DB:1001:A:H2'  | 23:DB:1002:G:O4'   | 2.12                     | 0.48              |
| 23:DB:1323:C:OP1  | 40:DS:82:MET:HE2   | 2.13                     | 0.48              |
| 23:DB:1790:C:P    | 25:DC:219:VAL:HB   | 2.54                     | 0.48              |
| 23:DB:1799:G:N7   | 25:DC:178:GLY:CA   | 2.72                     | 0.48              |
| 23:DB:2488:G:O2'  | 23:DB:2489:U:H5'   | 2.12                     | 0.48              |
| 23:DB:2893:A:H4'  | 23:DB:2894:G:O5'   | 2.12                     | 0.48              |
| 24:DV:29:ILE:HG22 | 24:DV:90:ASP:HA    | 1.94                     | 0.48              |
| 24:DV:70:ILE:HD12 | 24:DV:71:LYS:N     | 2.23                     | 0.48              |
| 25:DC:94:LEU:HD13 | 25:DC:100:ARG:HG3  | 1.94                     | 0.48              |
| 25:DC:124:LYS:HB2 | 25:DC:125:PRO:HD2  | 1.93                     | 0.48              |
| 26:DD:14:ILE:HG23 | 26:DD:19:GLY:HA3   | 1.95                     | 0.48              |
| 26:DD:46:ARG:H    | 26:DD:82:PHE:HA    | 1.78                     | 0.48              |
| 27:DE:4:VAL:HA    | 27:DE:14:VAL:HG13  | 1.94                     | 0.48              |
| 27:DE:132:LYS:H   | 27:DE:134:LEU:CD1  | 2.26                     | 0.48              |
| 32:DK:103:VAL:O   | 32:DK:104:THR:HG23 | 2.13                     | 0.48              |
| 44:DX:28:LEU:HD13 | 44:DX:42:LEU:HD21  | 1.94                     | 0.48              |
| 44:DX:28:LEU:HA   | 44:DX:30:MET:HE2   | 1.95                     | 0.48              |
| 46:DZ:30:HIS:HB3  | 46:DZ:32:LEU:HD23  | 1.95                     | 0.48              |
| 1:AA:79:G:H2'     | 1:AA:80:A:H8       | 1.74                     | 0.48              |
| 1:AA:319:G:O2'    | 1:AA:320:A:H5'     | 2.14                     | 0.48              |
| 1:AA:408:A:O5'    | 3:AD:109:THR:HG21  | 2.12                     | 0.48              |
| 1:AA:1021:A:H2'   | 1:AA:1022:A:O4'    | 2.13                     | 0.48              |
| 1:AA:1082:A:O2'   | 1:AA:1083:U:H5'    | 2.13                     | 0.48              |
| 1:AA:1225:A:H4'   | 18:AS:77:ARG:HH22  | 1.77                     | 0.48              |
| 1:AA:1247:U:O2'   | 1:AA:1248:A:H5'    | 2.13                     | 0.48              |
| 2:AC:122:GLN:HE22 | 2:AC:136:ALA:HB1   | 1.79                     | 0.48              |
| 2:AC:141:MET:CE   | 2:AC:147:GLY:H     | 2.25                     | 0.48              |
| 3:AD:160:LEU:HD22 | 3:AD:161:ALA:N     | 2.29                     | 0.48              |
| 6:AG:30:MET:HA    | 6:AG:38:ALA:HB2    | 1.94                     | 0.48              |
| 8:AI:33:SER:C     | 8:AI:35:GLU:H      | 2.21                     | 0.48              |
| 23:BB:231:A:H3'   | 23:BB:232:G:C8     | 2.48                     | 0.48              |
| 23:BB:582:A:H2'   | 23:BB:583:G:C8     | 2.47                     | 0.48              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:773:U:H4'    | 25:BC:47:ARG:HB3   | 1.94                     | 0.48              |
| 23:BB:850:U:H2'    | 23:BB:851:C:C6     | 2.48                     | 0.48              |
| 23:BB:1080:A:O2'   | 52:BI:126:ARG:HB2  | 2.13                     | 0.48              |
| 23:BB:1151:A:H4'   | 38:BQ:80:ASN:OD1   | 2.12                     | 0.48              |
| 23:BB:1230:A:H2'   | 23:BB:1231:U:H6    | 1.78                     | 0.48              |
| 23:BB:1439:A:C8    | 23:BB:1440:U:C6    | 3.01                     | 0.48              |
| 23:BB:1463:C:H2'   | 23:BB:1464:G:C8    | 2.48                     | 0.48              |
| 23:BB:1726:C:H2'   | 23:BB:1727:C:C6    | 2.49                     | 0.48              |
| 23:BB:2803:G:H2'   | 23:BB:2804:U:H6    | 1.79                     | 0.48              |
| 23:BB:2893:A:H4'   | 23:BB:2894:G:O5'   | 2.12                     | 0.48              |
| 24:BV:76:ASP:CB    | 34:BM:136:MET:HG3  | 2.44                     | 0.48              |
| 25:BC:16:VAL:CA    | 25:BC:17:LYS:HZ3   | 2.24                     | 0.48              |
| 25:BC:198:GLU:C    | 25:BC:200:MET:N    | 2.70                     | 0.48              |
| 25:BC:260:LYS:C    | 25:BC:262:THR:H    | 2.21                     | 0.48              |
| 26:BD:16:THR:HG23  | 26:BD:17:GLU:N     | 2.13                     | 0.48              |
| 26:BD:119:ALA:HB1  | 26:BD:123:LYS:HB2  | 1.96                     | 0.48              |
| 27:BE:108:ILE:HD12 | 27:BE:108:ILE:N    | 2.28                     | 0.48              |
| 28:BF:103:ILE:HG13 | 28:BF:104:THR:N    | 2.27                     | 0.48              |
| 28:BF:133:GLU:HG3  | 28:BF:134:GLN:H    | 1.77                     | 0.48              |
| 32:BK:23:LYS:CG    | 32:BK:24:VAL:N     | 2.77                     | 0.48              |
| 34:BM:76:LYS:HA    | 34:BM:86:LYS:HD3   | 1.94                     | 0.48              |
| 35:BN:77:ALA:HA    | 35:BN:80:PHE:CE2   | 2.48                     | 0.48              |
| 36:BO:10:ARG:HH11  | 36:BO:10:ARG:HG3   | 1.78                     | 0.48              |
| 37:BP:2:ASN:H      | 37:BP:2:ASN:ND2    | 2.06                     | 0.48              |
| 37:BP:47:ILE:HG23  | 37:BP:63:ILE:HA    | 1.95                     | 0.48              |
| 38:BQ:71:ASN:HD21  | 38:BQ:109:VAL:HG11 | 1.78                     | 0.48              |
| 39:BR:1:MET:HA     | 39:BR:46:GLU:HG3   | 1.94                     | 0.48              |
| 39:BR:18:GLN:CB    | 39:BR:99:THR:HA    | 2.42                     | 0.48              |
| 39:BR:85:LYS:C     | 39:BR:87:GLN:N     | 2.71                     | 0.48              |
| 40:BS:42:LYS:O     | 40:BS:46:LEU:HG    | 2.14                     | 0.48              |
| 43:BW:16:GLU:HA    | 43:BW:18:LYS:NZ    | 2.28                     | 0.48              |
| 46:BZ:35:ASP:O     | 46:BZ:42:PRO:HB3   | 2.13                     | 0.48              |
| 48:B1:46:VAL:HG22  | 48:B1:47:ILE:H     | 1.76                     | 0.48              |
| 50:B3:14:LYS:O     | 50:B3:21:PHE:HB3   | 2.13                     | 0.48              |
| 52:BI:79:LEU:HD11  | 52:BI:131:THR:OG1  | 2.12                     | 0.48              |
| 1:CA:8:A:C6        | 3:CD:205:LYS:HA    | 2.47                     | 0.48              |
| 1:CA:182:A:H1'     | 1:CA:183:C:C5      | 2.48                     | 0.48              |
| 1:CA:236:A:H2'     | 1:CA:237:G:H8      | 1.78                     | 0.48              |
| 1:CA:255:G:H5'     | 16:CQ:17:GLU:O     | 2.13                     | 0.48              |
| 1:CA:319:G:O2'     | 1:CA:320:A:H5'     | 2.13                     | 0.48              |
| 1:CA:505:G:H5'     | 1:CA:534:U:H2'     | 1.94                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:513:C:H2'     | 1:CA:514:C:H6      | 1.79                     | 0.48              |
| 1:CA:560:A:H4'     | 1:CA:561:U:H5''    | 1.94                     | 0.48              |
| 1:CA:634:C:O2'     | 1:CA:635:A:H5'     | 2.13                     | 0.48              |
| 1:CA:1093:A:P      | 6:CG:3:ARG:HH22    | 2.36                     | 0.48              |
| 4:CE:39:GLY:HA3    | 4:CE:116:VAL:HB    | 1.95                     | 0.48              |
| 15:CP:22:ALA:HB2   | 15:CP:32:PHE:HA    | 1.94                     | 0.48              |
| 16:CQ:68:LYS:C     | 16:CQ:70:LYS:H     | 2.21                     | 0.48              |
| 19:CT:56:ILE:O     | 19:CT:60:GLN:HG2   | 2.13                     | 0.48              |
| 20:CB:132:GLU:HG2  | 20:CB:135:MET:HE2  | 1.95                     | 0.48              |
| 23:DB:197:A:H4'    | 23:DB:2069:G:OP2   | 2.12                     | 0.48              |
| 23:DB:455:C:N4     | 23:DB:472:A:H2'    | 2.28                     | 0.48              |
| 23:DB:974:G:H4'    | 39:DR:83:TYR:OH    | 2.13                     | 0.48              |
| 23:DB:1236:G:C2'   | 23:DB:1237:A:OP2   | 2.61                     | 0.48              |
| 23:DB:1287:A:H3'   | 23:DB:1288:G:N2    | 2.28                     | 0.48              |
| 23:DB:2063:C:O2    | 23:DB:2450:A:N1    | 2.46                     | 0.48              |
| 23:DB:2378:A:C2'   | 23:DB:2379:G:H5'   | 2.43                     | 0.48              |
| 23:DB:2484:G:H1'   | 34:DM:119:LEU:CD1  | 2.42                     | 0.48              |
| 23:DB:2751:G:OP2   | 29:DG:3:VAL:HB     | 2.14                     | 0.48              |
| 23:DB:2873:A:N3    | 35:DN:6:SER:HA     | 2.28                     | 0.48              |
| 25:DC:38:LYS:HG3   | 25:DC:39:SER:H     | 1.79                     | 0.48              |
| 25:DC:216:ARG:HB3  | 25:DC:217:PRO:HD2  | 1.94                     | 0.48              |
| 25:DC:261:ARG:HG2  | 25:DC:261:ARG:NH1  | 2.28                     | 0.48              |
| 27:DE:112:LEU:HD12 | 27:DE:115:GLN:HE22 | 1.78                     | 0.48              |
| 29:DG:84:LYS:HE2   | 29:DG:163:TYR:CD1  | 2.48                     | 0.48              |
| 31:DJ:32:LEU:O     | 31:DJ:36:LEU:HD13  | 2.13                     | 0.48              |
| 31:DJ:121:LYS:N    | 31:DJ:121:LYS:CE   | 2.74                     | 0.48              |
| 32:DK:33:ALA:CB    | 32:DK:39:ILE:HD11  | 2.44                     | 0.48              |
| 35:DN:32:GLU:HA    | 35:DN:115:LEU:HD21 | 1.95                     | 0.48              |
| 35:DN:97:ILE:HG23  | 35:DN:113:ILE:HD11 | 1.95                     | 0.48              |
| 39:DR:67:GLY:H     | 39:DR:98:ILE:H     | 1.60                     | 0.48              |
| 39:DR:69:GLY:HA2   | 39:DR:96:VAL:CA    | 2.43                     | 0.48              |
| 42:DU:4:ILE:HD13   | 42:DU:4:ILE:C      | 2.38                     | 0.48              |
| 43:DW:42:THR:HB    | 43:DW:75:ASN:ND2   | 2.28                     | 0.48              |
| 49:D2:34:ARG:NH1   | 49:D2:35:ARG:NH1   | 2.61                     | 0.48              |
| 1:AA:418:C:H2'     | 1:AA:419:C:H6      | 1.78                     | 0.48              |
| 1:AA:554:A:H2'     | 1:AA:555:U:C6      | 2.49                     | 0.48              |
| 1:AA:708:C:H2'     | 1:AA:709:U:C6      | 2.48                     | 0.48              |
| 1:AA:926:G:N2      | 1:AA:1505:G:H2'    | 2.29                     | 0.48              |
| 2:AC:66:THR:HA     | 2:AC:101:ASN:O     | 2.14                     | 0.48              |
| 4:AE:114:LEU:C     | 4:AE:116:VAL:H     | 2.21                     | 0.48              |
| 5:AF:9:MET:HA      | 5:AF:58:HIS:O      | 2.13                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:AF:67:PRO:O      | 5:AF:70:VAL:HG22   | 2.13                     | 0.48              |
| 10:AK:88:PRO:HD3   | 21:AU:28:LEU:CD1   | 2.41                     | 0.48              |
| 21:AU:13:VAL:CG1   | 21:AU:14:ALA:H     | 2.17                     | 0.48              |
| 22:BA:52:A:H3'     | 22:BA:53:A:H8      | 1.77                     | 0.48              |
| 23:BB:62:U:H3'     | 23:BB:63:A:C8      | 2.49                     | 0.48              |
| 23:BB:685:A:H1'    | 23:BB:688:U:O4     | 2.13                     | 0.48              |
| 23:BB:843:G:H2'    | 23:BB:844:A:C8     | 2.48                     | 0.48              |
| 23:BB:970:U:H2'    | 23:BB:971:G:H8     | 1.78                     | 0.48              |
| 23:BB:1011:G:O2'   | 23:BB:1013:C:H5''  | 2.13                     | 0.48              |
| 23:BB:1312:U:H4'   | 23:BB:1313:U:O5'   | 2.12                     | 0.48              |
| 23:BB:1313:U:O2    | 23:BB:1313:U:H2'   | 2.12                     | 0.48              |
| 23:BB:1407:G:H2'   | 23:BB:1408:G:H8    | 1.78                     | 0.48              |
| 23:BB:2316:G:H2'   | 23:BB:2317:A:H8    | 1.78                     | 0.48              |
| 23:BB:2468:A:H2'   | 23:BB:2476:A:C6    | 2.48                     | 0.48              |
| 23:BB:2544:G:H2'   | 23:BB:2545:G:H8    | 1.78                     | 0.48              |
| 24:BV:57:TYR:HA    | 24:BV:74:ALA:HB3   | 1.95                     | 0.48              |
| 24:BV:75:GLN:CD    | 34:BM:136:MET:HE2  | 2.39                     | 0.48              |
| 25:BC:129:LEU:HD22 | 25:BC:133:ASN:HB2  | 1.94                     | 0.48              |
| 25:BC:155:ARG:HH21 | 25:BC:155:ARG:HG2  | 1.79                     | 0.48              |
| 25:BC:171:VAL:HA   | 25:BC:183:VAL:O    | 2.13                     | 0.48              |
| 25:BC:204:LEU:HD11 | 25:BC:211:ARG:HH11 | 1.79                     | 0.48              |
| 25:BC:216:ARG:HB3  | 25:BC:217:PRO:CD   | 2.43                     | 0.48              |
| 25:BC:220:ARG:HH11 | 25:BC:220:ARG:HG3  | 1.78                     | 0.48              |
| 28:BF:135:ILE:C    | 28:BF:137:PHE:N    | 2.71                     | 0.48              |
| 31:BJ:132:HIS:HB3  | 31:BJ:136:GLN:HE22 | 1.78                     | 0.48              |
| 33:BL:79:LEU:H     | 33:BL:79:LEU:CD1   | 2.26                     | 0.48              |
| 34:BM:43:ALA:C     | 34:BM:45:GLN:N     | 2.67                     | 0.48              |
| 37:BP:25:VAL:CG2   | 37:BP:49:ILE:HD11  | 2.44                     | 0.48              |
| 44:BX:10:SER:C     | 44:BX:12:GLU:H     | 2.22                     | 0.48              |
| 49:B2:3:ARG:HB3    | 49:B2:5:PHE:CE1    | 2.48                     | 0.48              |
| 1:CA:157:U:O2'     | 1:CA:158:G:H5'     | 2.13                     | 0.48              |
| 1:CA:399:G:H2'     | 1:CA:400:C:H6      | 1.77                     | 0.48              |
| 1:CA:448:A:O2'     | 1:CA:449:G:H5'     | 2.12                     | 0.48              |
| 1:CA:600:A:H2'     | 1:CA:601:G:C8      | 2.48                     | 0.48              |
| 1:CA:608:A:H2'     | 1:CA:609:A:O4'     | 2.14                     | 0.48              |
| 1:CA:692:U:H2'     | 1:CA:694:A:OP2     | 2.14                     | 0.48              |
| 1:CA:1250:A:H4'    | 8:CI:69:GLY:N      | 2.17                     | 0.48              |
| 1:CA:1309:G:H1'    | 12:CM:72:ILE:HG13  | 1.95                     | 0.48              |
| 1:CA:1349:A:H1'    | 1:CA:1374:A:N6     | 2.28                     | 0.48              |
| 1:CA:1411:C:H2'    | 1:CA:1412:C:C6     | 2.49                     | 0.48              |
| 1:CA:1499:A:O2'    | 1:CA:1500:A:H5'    | 2.14                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:CD:25:ARG:HG3   | 3:CD:25:ARG:O      | 2.13                     | 0.48              |
| 9:CJ:15:HIS:O     | 9:CJ:18:ILE:HG22   | 2.13                     | 0.48              |
| 12:CM:89:ARG:CB   | 12:CM:96:VAL:HG22  | 2.44                     | 0.48              |
| 15:CP:54:LEU:HA   | 15:CP:57:ILE:CG2   | 2.43                     | 0.48              |
| 16:CQ:45:VAL:HG11 | 16:CQ:60:ILE:HG21  | 1.96                     | 0.48              |
| 19:CT:50:PHE:O    | 19:CT:53:MET:HG3   | 2.13                     | 0.48              |
| 23:DB:455:C:H42   | 23:DB:472:A:H2'    | 1.77                     | 0.48              |
| 23:DB:562:U:C4    | 23:DB:2036:C:O4'   | 2.67                     | 0.48              |
| 23:DB:856:G:H2'   | 23:DB:857:G:C8     | 2.48                     | 0.48              |
| 23:DB:1213:A:N1   | 23:DB:1237:A:H1'   | 2.27                     | 0.48              |
| 23:DB:1244:A:O2'  | 23:DB:1245:G:H5'   | 2.13                     | 0.48              |
| 23:DB:1268:A:H2'  | 23:DB:1269:A:O4'   | 2.13                     | 0.48              |
| 23:DB:1312:U:H4'  | 23:DB:1313:U:O5'   | 2.12                     | 0.48              |
| 23:DB:1511:G:H2'  | 23:DB:1512:C:H6    | 1.77                     | 0.48              |
| 23:DB:1818:U:OP1  | 25:DC:155:ARG:HA   | 2.12                     | 0.48              |
| 23:DB:2226:C:H2'  | 23:DB:2227:A:O4'   | 2.13                     | 0.48              |
| 23:DB:2544:G:H2'  | 23:DB:2545:G:H8    | 1.77                     | 0.48              |
| 23:DB:2834:G:H2'  | 23:DB:2879:A:N6    | 2.28                     | 0.48              |
| 55:DB:3317:HOH:O  | 26:DD:152:PRO:HG2  | 2.12                     | 0.48              |
| 25:DC:225:ASN:N   | 25:DC:226:PRO:HD3  | 2.29                     | 0.48              |
| 26:DD:62:LYS:CB   | 26:DD:63:PRO:HD3   | 2.43                     | 0.48              |
| 27:DE:149:ILE:CD1 | 27:DE:188:MET:HB2  | 2.44                     | 0.48              |
| 28:DF:56:LEU:CA   | 28:DF:59:ILE:HG22  | 2.42                     | 0.48              |
| 33:DL:79:LEU:HD11 | 33:DL:112:LEU:HD23 | 1.96                     | 0.48              |
| 36:DO:29:HIS:HB3  | 36:DO:36:TYR:HB2   | 1.95                     | 0.48              |
| 37:DP:86:LYS:C    | 37:DP:87:ARG:HG3   | 2.37                     | 0.48              |
| 40:DS:27:LYS:N    | 40:DS:27:LYS:HD2   | 2.29                     | 0.48              |
| 41:DT:65:GLY:HA3  | 41:DT:76:ARG:HH21  | 1.78                     | 0.48              |
| 44:DX:26:PHE:H    | 44:DX:26:PHE:HD1   | 1.60                     | 0.48              |
| 44:DX:47:ARG:HA   | 44:DX:50:VAL:HG23  | 1.95                     | 0.48              |
| 45:DY:2:LYS:H     | 45:DY:37:ARG:HB3   | 1.78                     | 0.48              |
| 52:DI:17:ALA:O    | 52:DI:18:ASN:CB    | 2.61                     | 0.48              |
| 1:AA:90:C:H2'     | 1:AA:91:U:C6       | 2.47                     | 0.48              |
| 1:AA:766:A:H2'    | 1:AA:767:A:O4'     | 2.13                     | 0.48              |
| 1:AA:1038:C:H2'   | 1:AA:1039:G:H8     | 1.78                     | 0.48              |
| 1:AA:1318:A:H4'   | 18:AS:9:PHE:CD1    | 2.49                     | 0.48              |
| 8:AI:38:PHE:O     | 8:AI:39:GLY:C      | 2.55                     | 0.48              |
| 13:AN:27:LYS:HD2  | 13:AN:27:LYS:C     | 2.38                     | 0.48              |
| 15:AP:28:ARG:HG3  | 15:AP:29:ASN:ND2   | 2.29                     | 0.48              |
| 18:AS:51:HIS:C    | 18:AS:53:GLY:H     | 2.21                     | 0.48              |
| 21:AU:3:ILE:CA    | 21:AU:19:LYS:HG2   | 2.35                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:AU:31:VAL:O    | 21:AU:32:ARG:C    | 2.56                     | 0.48              |
| 21:AU:37:TYR:C    | 21:AU:40:PRO:HD2  | 2.38                     | 0.48              |
| 22:BA:63:C:H2'    | 22:BA:64:G:H8     | 1.79                     | 0.48              |
| 23:BB:39:G:O2'    | 23:BB:40:U:H5'    | 2.14                     | 0.48              |
| 23:BB:130:C:O2'   | 23:BB:131:A:H5'   | 2.12                     | 0.48              |
| 23:BB:142:A:H2'   | 23:BB:143:C:H6    | 1.79                     | 0.48              |
| 23:BB:276:U:O2'   | 23:BB:277:G:H5'   | 2.14                     | 0.48              |
| 23:BB:363:G:H2'   | 23:BB:364:C:H6    | 1.78                     | 0.48              |
| 23:BB:572:A:H5''  | 23:BB:573:U:OP2   | 2.12                     | 0.48              |
| 23:BB:909:A:H2'   | 23:BB:912:C:H5    | 1.79                     | 0.48              |
| 23:BB:1299:G:C4'  | 23:BB:1301:A:H1'  | 2.40                     | 0.48              |
| 23:BB:1579:A:H2'  | 23:BB:1580:A:H8   | 1.78                     | 0.48              |
| 23:BB:1599:U:H2'  | 23:BB:1600:C:C6   | 2.48                     | 0.48              |
| 23:BB:1817:G:OP1  | 25:BC:62:ARG:NH2  | 2.46                     | 0.48              |
| 23:BB:2053:G:OP1  | 26:BD:149:ASN:O   | 2.31                     | 0.48              |
| 23:BB:2260:C:O2'  | 23:BB:2261:C:H5'  | 2.14                     | 0.48              |
| 23:BB:2308:G:N3   | 23:BB:2308:G:H3'  | 2.28                     | 0.48              |
| 23:BB:2575:C:C5'  | 26:BD:149:ASN:N   | 2.74                     | 0.48              |
| 23:BB:2722:G:H2'  | 23:BB:2723:C:C6   | 2.49                     | 0.48              |
| 23:BB:2812:G:H2'  | 23:BB:2813:A:O4'  | 2.13                     | 0.48              |
| 24:BV:79:ARG:CZ   | 24:BV:79:ARG:HB3  | 2.43                     | 0.48              |
| 25:BC:155:ARG:NH2 | 25:BC:155:ARG:HG2 | 2.29                     | 0.48              |
| 26:BD:106:LYS:HZ2 | 26:BD:208:LYS:HD3 | 1.78                     | 0.48              |
| 27:BE:75:SER:C    | 27:BE:77:ILE:H    | 2.22                     | 0.48              |
| 29:BG:174:LYS:HD2 | 29:BG:174:LYS:N   | 2.29                     | 0.48              |
| 31:BJ:15:TRP:HB3  | 31:BJ:53:TYR:CE2  | 2.48                     | 0.48              |
| 33:BL:88:GLY:C    | 33:BL:90:VAL:H    | 2.20                     | 0.48              |
| 38:BQ:88:GLU:HA   | 39:BR:53:PHE:CG   | 2.48                     | 0.48              |
| 40:BS:32:ALA:O    | 40:BS:33:LEU:HD13 | 2.14                     | 0.48              |
| 41:BT:6:ARG:HG3   | 41:BT:10:VAL:HG13 | 1.95                     | 0.48              |
| 41:BT:30:ILE:CG2  | 41:BT:85:VAL:HG22 | 2.43                     | 0.48              |
| 46:BZ:30:HIS:O    | 46:BZ:48:GLN:NE2  | 2.47                     | 0.48              |
| 46:BZ:50:ASP:CA   | 46:BZ:53:THR:HG22 | 2.43                     | 0.48              |
| 1:CA:16:A:N1      | 1:CA:919:A:C2     | 2.82                     | 0.48              |
| 1:CA:627:G:H2'    | 1:CA:628:G:H8     | 1.78                     | 0.48              |
| 1:CA:964:A:H2'    | 1:CA:965:U:H5''   | 1.95                     | 0.48              |
| 1:CA:1250:A:O2'   | 1:CA:1251:A:O4'   | 2.31                     | 0.48              |
| 2:CC:119:ILE:HD12 | 2:CC:132:ALA:HB1  | 1.95                     | 0.48              |
| 3:CD:44:LYS:HZ2   | 3:CD:45:PRO:C     | 2.22                     | 0.48              |
| 11:CL:100:ALA:C   | 11:CL:103:CYS:HG  | 2.21                     | 0.48              |
| 16:CQ:25:GLU:HA   | 16:CQ:40:THR:HA   | 1.96                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:CQ:80:LYS:H     | 16:CQ:80:LYS:CD    | 2.26                     | 0.48              |
| 20:CB:42:LEU:C     | 20:CB:44:LYS:H     | 2.20                     | 0.48              |
| 20:CB:85:SER:O     | 20:CB:86:CYS:HB2   | 2.12                     | 0.48              |
| 23:DB:673:C:O2'    | 23:DB:674:G:H5'    | 2.13                     | 0.48              |
| 23:DB:723:C:H2'    | 23:DB:724:U:H6     | 1.79                     | 0.48              |
| 23:DB:1178:C:C2    | 23:DB:1179:G:N7    | 2.81                     | 0.48              |
| 23:DB:1299:G:H4'   | 23:DB:1301:A:C1'   | 2.42                     | 0.48              |
| 23:DB:1322:A:C2'   | 23:DB:1323:C:H5'   | 2.44                     | 0.48              |
| 23:DB:1581:G:O2'   | 23:DB:1582:C:H5'   | 2.13                     | 0.48              |
| 23:DB:1726:C:H2'   | 23:DB:1727:C:C6    | 2.49                     | 0.48              |
| 23:DB:2563:U:H2'   | 23:DB:2565:A:OP2   | 2.13                     | 0.48              |
| 23:DB:2568:U:H2'   | 23:DB:2569:G:O4'   | 2.14                     | 0.48              |
| 23:DB:2803:G:H2'   | 23:DB:2804:U:H6    | 1.79                     | 0.48              |
| 23:DB:2840:C:H2'   | 23:DB:2841:C:C6    | 2.48                     | 0.48              |
| 25:DC:140:VAL:HG11 | 25:DC:163:ILE:CD1  | 2.42                     | 0.48              |
| 27:DE:15:SER:CB    | 27:DE:196:VAL:HG22 | 2.41                     | 0.48              |
| 27:DE:49:ARG:HB2   | 27:DE:51:GLU:CD    | 2.38                     | 0.48              |
| 27:DE:147:LEU:HD12 | 27:DE:147:LEU:N    | 2.27                     | 0.48              |
| 27:DE:152:GLU:OE2  | 27:DE:188:MET:HA   | 2.13                     | 0.48              |
| 28:DF:140:ILE:C    | 28:DF:142:TYR:H    | 2.21                     | 0.48              |
| 30:DH:90:LEU:HD13  | 30:DH:122:LEU:O    | 2.14                     | 0.48              |
| 30:DH:135:HIS:CG   | 30:DH:136:SER:N    | 2.81                     | 0.48              |
| 35:DN:126:ALA:C    | 35:DN:127:GLU:HG2  | 2.39                     | 0.48              |
| 37:DP:48:ALA:HB3   | 37:DP:64:SER:HB3   | 1.94                     | 0.48              |
| 39:DR:18:GLN:CD    | 39:DR:18:GLN:H     | 2.21                     | 0.48              |
| 41:DT:2:ILE:HG12   | 41:DT:3:ARG:N      | 2.27                     | 0.48              |
| 46:DZ:62:LYS:CA    | 46:DZ:65:ASN:HD21  | 2.26                     | 0.48              |
| 48:D1:4:ILE:HG23   | 48:D1:4:ILE:O      | 2.13                     | 0.48              |
| 1:AA:429:U:H3'     | 3:AD:8:LEU:HD23    | 1.96                     | 0.48              |
| 1:AA:869:G:H4'     | 1:AA:872:A:C8      | 2.49                     | 0.48              |
| 1:AA:978:A:O2'     | 1:AA:1322:C:H5     | 1.96                     | 0.48              |
| 1:AA:999:C:O2'     | 1:AA:1000:A:H5'    | 2.13                     | 0.48              |
| 1:AA:1025:U:H5''   | 1:AA:1026:G:OP1    | 2.14                     | 0.48              |
| 1:AA:1149:C:H2'    | 1:AA:1150:A:C8     | 2.48                     | 0.48              |
| 2:AC:90:VAL:HA     | 2:AC:93:ILE:HG21   | 1.95                     | 0.48              |
| 14:AO:54:GLY:O     | 14:AO:58:MET:HG2   | 2.13                     | 0.48              |
| 18:AS:4:LEU:CA     | 18:AS:5:LYS:HE3    | 2.43                     | 0.48              |
| 18:AS:18:VAL:HB    | 18:AS:43:MET:HE3   | 1.96                     | 0.48              |
| 18:AS:46:LEU:O     | 18:AS:60:PHE:HA    | 2.12                     | 0.48              |
| 23:BB:231:A:H3'    | 23:BB:232:G:H8     | 1.79                     | 0.48              |
| 23:BB:306:U:H2'    | 23:BB:307:G:O4'    | 2.13                     | 0.48              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BB:720:U:H2'   | 23:BB:721:A:H8    | 1.78                     | 0.48              |
| 23:BB:1017:G:H2'  | 23:BB:1018:U:C6   | 2.49                     | 0.48              |
| 23:BB:1079:C:O2'  | 52:BI:133:ARG:NH2 | 2.46                     | 0.48              |
| 23:BB:1332:G:N3   | 23:BB:1332:G:H2'  | 2.29                     | 0.48              |
| 23:BB:1355:G:O2'  | 23:BB:1356:G:H5'  | 2.14                     | 0.48              |
| 23:BB:1688:U:O2   | 23:BB:1700:A:H5'  | 2.13                     | 0.48              |
| 23:BB:2092:U:H4'  | 23:BB:2093:G:O5'  | 2.14                     | 0.48              |
| 23:BB:2180:U:H2'  | 23:BB:2181:U:C5   | 2.48                     | 0.48              |
| 23:BB:2307:G:H2'  | 23:BB:2307:G:N3   | 2.29                     | 0.48              |
| 23:BB:2530:A:H61  | 29:BG:155:PRO:HG3 | 1.78                     | 0.48              |
| 23:BB:2593:U:O2'  | 23:BB:2594:C:H5'  | 2.13                     | 0.48              |
| 23:BB:2645:G:H4'  | 23:BB:2732:G:H2'  | 1.96                     | 0.48              |
| 23:BB:2776:A:H4'  | 23:BB:2777:G:O5'  | 2.13                     | 0.48              |
| 24:BV:9:ARG:HB2   | 24:BV:39:ALA:O    | 2.13                     | 0.48              |
| 25:BC:71:ASP:O    | 25:BC:73:ILE:N    | 2.46                     | 0.48              |
| 26:BD:2:ILE:HG22  | 26:BD:204:LYS:HG3 | 1.95                     | 0.48              |
| 29:BG:114:HIS:HB2 | 29:BG:150:TYR:HE2 | 1.79                     | 0.48              |
| 30:BH:7:ASP:O     | 30:BH:9:VAL:HG23  | 2.13                     | 0.48              |
| 30:BH:7:ASP:OD1   | 30:BH:35:LYS:HB3  | 2.14                     | 0.48              |
| 30:BH:66:ASN:C    | 30:BH:68:ARG:H    | 2.22                     | 0.48              |
| 34:BM:73:ILE:CD1  | 34:BM:92:TRP:H    | 2.25                     | 0.48              |
| 35:BN:2:ARG:O     | 35:BN:3:HIS:CB    | 2.62                     | 0.48              |
| 35:BN:7:GLY:O     | 35:BN:8:ARG:CB    | 2.61                     | 0.48              |
| 35:BN:16:HIS:O    | 35:BN:20:MET:HG2  | 2.13                     | 0.48              |
| 37:BP:50:ARG:NH1  | 37:BP:62:LYS:HB3  | 2.29                     | 0.48              |
| 37:BP:52:ARG:N    | 37:BP:60:VAL:HG21 | 2.29                     | 0.48              |
| 39:BR:17:GLY:C    | 39:BR:18:GLN:HG2  | 2.39                     | 0.48              |
| 39:BR:41:ILE:O    | 39:BR:54:VAL:HG22 | 2.14                     | 0.48              |
| 39:BR:45:GLU:HA   | 39:BR:50:GLY:HA2  | 1.95                     | 0.48              |
| 39:BR:71:LYS:O    | 39:BR:94:THR:HA   | 2.13                     | 0.48              |
| 43:BW:28:GLU:C    | 43:BW:30:VAL:H    | 2.21                     | 0.48              |
| 46:BZ:64:PHE:C    | 46:BZ:67:PRO:HD2  | 2.39                     | 0.48              |
| 47:B0:36:LYS:HZ3  | 47:B0:41:HIS:HA   | 1.78                     | 0.48              |
| 51:B4:31:PRO:O    | 51:B4:32:LYS:C    | 2.56                     | 0.48              |
| 1:CA:123:U:H5''   | 1:CA:311:C:O2'    | 2.12                     | 0.48              |
| 1:CA:140:U:H2'    | 1:CA:141:G:C8     | 2.48                     | 0.48              |
| 1:CA:218:U:H2'    | 1:CA:219:U:H6     | 1.78                     | 0.48              |
| 1:CA:280:C:O2     | 16:CQ:39:ARG:HG3  | 2.13                     | 0.48              |
| 1:CA:840:C:C2     | 1:CA:842:U:H4'    | 2.49                     | 0.48              |
| 1:CA:1240:U:P     | 6:CG:115:MET:H    | 2.37                     | 0.48              |
| 6:CG:55:LYS:HG3   | 6:CG:56:SER:N     | 2.28                     | 0.48              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:CI:112:ARG:HD2   | 13:CN:100:TRP:OXT  | 2.13                     | 0.48              |
| 9:CJ:77:VAL:O      | 9:CJ:78:GLU:C      | 2.56                     | 0.48              |
| 10:CK:30:ILE:HG22  | 10:CK:45:THR:HB    | 1.95                     | 0.48              |
| 11:CL:100:ALA:O    | 11:CL:101:LEU:C    | 2.56                     | 0.48              |
| 14:CO:10:ILE:HD11  | 14:CO:29:ALA:HB1   | 1.94                     | 0.48              |
| 14:CO:84:LEU:HB3   | 14:CO:86:LEU:HD13  | 1.96                     | 0.48              |
| 20:CB:95:TRP:HZ3   | 20:CB:98:GLY:H     | 1.62                     | 0.48              |
| 21:CU:15:LEU:HA    | 21:CU:17:ARG:NH1   | 2.24                     | 0.48              |
| 22:DA:94:A:OP1     | 24:DV:19:ARG:HD3   | 2.13                     | 0.48              |
| 23:DB:274:C:H2'    | 23:DB:275:C:O4'    | 2.12                     | 0.48              |
| 23:DB:654:A:H2'    | 23:DB:655:A:C5'    | 2.33                     | 0.48              |
| 23:DB:859:G:O2'    | 23:DB:860:U:OP2    | 2.32                     | 0.48              |
| 23:DB:1313:U:H2'   | 23:DB:1313:U:O2    | 2.12                     | 0.48              |
| 23:DB:1791:A:H61   | 23:DB:1828:G:H1'   | 1.78                     | 0.48              |
| 23:DB:2000:C:O2'   | 23:DB:2001:C:H5'   | 2.14                     | 0.48              |
| 23:DB:2026:U:H2'   | 23:DB:2027:G:H8    | 1.77                     | 0.48              |
| 23:DB:2512:C:OP1   | 26:DD:128:ARG:N    | 2.47                     | 0.48              |
| 23:DB:2516:A:O2'   | 23:DB:2517:C:H5'   | 2.13                     | 0.48              |
| 23:DB:2633:G:C1'   | 26:DD:62:LYS:HG3   | 2.39                     | 0.48              |
| 23:DB:2862:G:H2'   | 23:DB:2863:C:H6    | 1.79                     | 0.48              |
| 24:DV:77:VAL:HG13  | 24:DV:89:ILE:CD1   | 2.44                     | 0.48              |
| 25:DC:53:ILE:HG23  | 25:DC:216:ARG:HB2  | 1.95                     | 0.48              |
| 25:DC:77:VAL:HG21  | 25:DC:109:LEU:HD23 | 1.95                     | 0.48              |
| 26:DD:175:LEU:HD21 | 26:DD:192:ALA:HB3  | 1.95                     | 0.48              |
| 26:DD:181:ASP:CG   | 26:DD:184:ARG:HB3  | 2.39                     | 0.48              |
| 27:DE:56:GLY:O     | 27:DE:57:LYS:HG3   | 2.14                     | 0.48              |
| 28:DF:136:ILE:O    | 28:DF:138:PRO:HD3  | 2.13                     | 0.48              |
| 33:DL:37:GLY:O     | 33:DL:38:GLN:HG3   | 2.14                     | 0.48              |
| 34:DM:43:ALA:HB3   | 34:DM:91:TYR:CE2   | 2.48                     | 0.48              |
| 34:DM:83:GLY:O     | 34:DM:84:LYS:HB2   | 2.12                     | 0.48              |
| 40:DS:72:THR:HG22  | 40:DS:106:VAL:O    | 2.13                     | 0.48              |
| 42:DU:48:VAL:HG13  | 42:DU:51:LEU:N     | 2.29                     | 0.48              |
| 43:DW:20:LEU:CD1   | 43:DW:31:LEU:HB2   | 2.44                     | 0.48              |
| 43:DW:43:LYS:O     | 43:DW:44:PHE:CB    | 2.60                     | 0.48              |
| 43:DW:67:LYS:CG    | 43:DW:71:LYS:HB2   | 2.36                     | 0.48              |
| 44:DX:19:LEU:C     | 44:DX:21:LEU:H     | 2.22                     | 0.48              |
| 51:D4:24:ARG:HE    | 51:D4:37:GLN:CA    | 2.26                     | 0.48              |
| 51:D4:30:GLU:CB    | 51:D4:33:HIS:HB2   | 2.41                     | 0.48              |
| 52:DI:70:THR:O     | 52:DI:70:THR:HG23  | 2.12                     | 0.48              |
| 1:AA:79:G:H2'      | 1:AA:80:A:O4'      | 2.14                     | 0.48              |
| 1:AA:147:G:H2'     | 1:AA:148:G:C8      | 2.48                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:340:U:H2'     | 1:AA:341:C:H6      | 1.79                     | 0.48              |
| 1:AA:397:A:H5'     | 1:AA:398:U:OP1     | 2.13                     | 0.48              |
| 1:AA:736:C:H2'     | 1:AA:737:C:H6      | 1.77                     | 0.48              |
| 1:AA:922:G:H2'     | 1:AA:923:A:H8      | 1.78                     | 0.48              |
| 1:AA:948:C:O2'     | 1:AA:949:A:H5'     | 2.14                     | 0.48              |
| 1:AA:1352:C:H2'    | 1:AA:1353:G:C8     | 2.49                     | 0.48              |
| 2:AC:133:MET:HE1   | 2:AC:165:GLU:HG2   | 1.95                     | 0.48              |
| 3:AD:2:ARG:HG3     | 3:AD:114:ARG:NH1   | 2.29                     | 0.48              |
| 10:AK:80:ASN:HD21  | 10:AK:107:THR:CG2  | 2.27                     | 0.48              |
| 11:AL:113:ARG:HA   | 11:AL:118:VAL:HG23 | 1.96                     | 0.48              |
| 11:AL:121:PRO:C    | 11:AL:123:ALA:H    | 2.21                     | 0.48              |
| 19:AT:19:HIS:O     | 19:AT:23:ARG:HG2   | 2.13                     | 0.48              |
| 20:AB:68:PHE:HA    | 20:AB:161:PHE:O    | 2.12                     | 0.48              |
| 23:BB:67:U:C4      | 23:BB:68:G:N7      | 2.82                     | 0.48              |
| 23:BB:712:G:H2'    | 23:BB:713:G:O4'    | 2.13                     | 0.48              |
| 23:BB:1059:G:N2    | 52:BI:130:GLY:HA3  | 2.29                     | 0.48              |
| 23:BB:1561:C:H2'   | 23:BB:1562:U:C6    | 2.49                     | 0.48              |
| 23:BB:1759:A:H4'   | 23:BB:2715:C:O4'   | 2.13                     | 0.48              |
| 23:BB:2000:C:O2'   | 23:BB:2001:C:H5'   | 2.14                     | 0.48              |
| 23:BB:2743:U:C3'   | 23:BB:2744:G:H5''  | 2.44                     | 0.48              |
| 23:BB:2795:C:O5'   | 23:BB:2795:C:H6    | 1.97                     | 0.48              |
| 24:BV:48:MET:HE3   | 24:BV:48:MET:O     | 2.14                     | 0.48              |
| 25:BC:51:ARG:HD3   | 25:BC:51:ARG:O     | 2.13                     | 0.48              |
| 25:BC:143:VAL:HG11 | 25:BC:173:LEU:HD11 | 1.95                     | 0.48              |
| 25:BC:171:VAL:HG21 | 25:BC:182:LYS:HD3  | 1.96                     | 0.48              |
| 25:BC:218:THR:HG22 | 25:BC:218:THR:O    | 2.13                     | 0.48              |
| 25:BC:226:PRO:HD3  | 25:BC:233:GLY:N    | 2.29                     | 0.48              |
| 26:BD:34:VAL:HG11  | 26:BD:71:ALA:CB    | 2.44                     | 0.48              |
| 26:BD:46:ARG:HD2   | 26:BD:80:TRP:CE2   | 2.49                     | 0.48              |
| 28:BF:136:ILE:C    | 28:BF:138:PRO:HD3  | 2.39                     | 0.48              |
| 30:BH:19:VAL:HG12  | 30:BH:20:ASN:N     | 2.28                     | 0.48              |
| 31:BJ:25:LEU:HD12  | 31:BJ:62:VAL:HG12  | 1.94                     | 0.48              |
| 33:BL:60:ARG:NH1   | 50:B3:11:LYS:HE2   | 2.27                     | 0.48              |
| 33:BL:110:VAL:HG23 | 33:BL:126:ARG:CB   | 2.43                     | 0.48              |
| 34:BM:20:LEU:CB    | 34:BM:38:ARG:HD3   | 2.43                     | 0.48              |
| 35:BN:102:PHE:N    | 35:BN:102:PHE:HD2  | 2.11                     | 0.48              |
| 36:BO:58:ILE:HG13  | 36:BO:63:LYS:HB3   | 1.94                     | 0.48              |
| 38:BQ:26:ALA:C     | 38:BQ:28:SER:H     | 2.22                     | 0.48              |
| 40:BS:28:LYS:HB3   | 40:BS:71:VAL:HG21  | 1.96                     | 0.48              |
| 42:BU:76:THR:O     | 42:BU:77:GLY:C     | 2.56                     | 0.48              |
| 45:BY:9:THR:HG23   | 45:BY:10:ARG:N     | 2.25                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 52:BI:75:ALA:HB2  | 52:BI:112:LYS:HE2 | 1.95                     | 0.48              |
| 1:CA:659:U:H2'    | 1:CA:660:C:C6     | 2.48                     | 0.48              |
| 1:CA:893:C:H2'    | 1:CA:894:G:H8     | 1.78                     | 0.48              |
| 1:CA:903:G:H2'    | 1:CA:904:U:C6     | 2.48                     | 0.48              |
| 1:CA:1116:U:O2'   | 1:CA:1117:A:H5'   | 2.13                     | 0.48              |
| 1:CA:1164:G:O2'   | 1:CA:1165:U:H5'   | 2.13                     | 0.48              |
| 1:CA:1287:A:H2'   | 1:CA:1288:A:H8    | 1.76                     | 0.48              |
| 1:CA:1390:U:H2'   | 1:CA:1391:U:C6    | 2.49                     | 0.48              |
| 1:CA:1516:G:H2'   | 1:CA:1518:A:OP2   | 2.13                     | 0.48              |
| 3:CD:33:ILE:O     | 3:CD:34:GLU:C     | 2.57                     | 0.48              |
| 4:CE:148:SER:HB2  | 4:CE:149:PRO:HD2  | 1.94                     | 0.48              |
| 6:CG:139:ASP:O    | 6:CG:142:ARG:HB3  | 2.14                     | 0.48              |
| 8:CI:33:SER:HB2   | 8:CI:36:GLN:CG    | 2.44                     | 0.48              |
| 9:CJ:37:ARG:HG2   | 9:CJ:37:ARG:NH1   | 2.29                     | 0.48              |
| 9:CJ:64:GLN:CB    | 13:CN:98:ALA:HB3  | 2.43                     | 0.48              |
| 10:CK:70:ALA:N    | 10:CK:73:VAL:HG22 | 2.29                     | 0.48              |
| 13:CN:40:ARG:CZ   | 18:CS:6:LYS:HB2   | 2.44                     | 0.48              |
| 16:CQ:60:ILE:HG12 | 16:CQ:72:TRP:HE3  | 1.78                     | 0.48              |
| 18:CS:56:HIS:N    | 18:CS:56:HIS:CD2  | 2.80                     | 0.48              |
| 23:DB:417:C:H2'   | 23:DB:418:C:H6    | 1.78                     | 0.48              |
| 23:DB:493:G:O2'   | 23:DB:494:G:H5'   | 2.14                     | 0.48              |
| 23:DB:851:C:H2'   | 23:DB:852:U:C6    | 2.49                     | 0.48              |
| 23:DB:955:U:H5'   | 23:DB:956:G:OP2   | 2.12                     | 0.48              |
| 23:DB:1407:G:H2'  | 23:DB:1408:G:H8   | 1.78                     | 0.48              |
| 23:DB:1727:C:H2'  | 23:DB:1728:C:H6   | 1.74                     | 0.48              |
| 23:DB:2105:U:H2'  | 23:DB:2106:U:C6   | 2.48                     | 0.48              |
| 23:DB:2800:A:H2'  | 23:DB:2801:G:C4'  | 2.43                     | 0.48              |
| 25:DC:212:TRP:CZ3 | 25:DC:217:PRO:HD3 | 2.49                     | 0.48              |
| 26:DD:48:ILE:CG2  | 26:DD:49:GLN:N    | 2.76                     | 0.48              |
| 30:DH:2:GLN:CB    | 30:DH:19:VAL:HA   | 2.43                     | 0.48              |
| 31:DJ:68:LYS:HD2  | 31:DJ:72:LYS:CB   | 2.43                     | 0.48              |
| 35:DN:2:ARG:NH1   | 35:DN:4:ARG:HH12  | 2.11                     | 0.48              |
| 36:DO:4:LYS:O     | 36:DO:7:ARG:HG2   | 2.12                     | 0.48              |
| 37:DP:85:VAL:O    | 37:DP:87:ARG:NE   | 2.46                     | 0.48              |
| 38:DQ:50:ARG:HH22 | 38:DQ:53:LYS:NZ   | 2.12                     | 0.48              |
| 42:DU:22:GLY:HA3  | 42:DU:35:VAL:CG2  | 2.43                     | 0.48              |
| 45:DY:3:THR:CA    | 45:DY:37:ARG:H    | 2.23                     | 0.48              |
| 45:DY:26:LEU:C    | 45:DY:28:LEU:N    | 2.71                     | 0.48              |
| 1:AA:267:C:OP2    | 16:AQ:68:LYS:HD2  | 2.14                     | 0.48              |
| 1:AA:363:A:OP2    | 11:AL:30:ARG:NH1  | 2.47                     | 0.48              |
| 1:AA:591:U:H2'    | 1:AA:592:G:C8     | 2.48                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1037:C:H2'   | 1:AA:1038:C:C6     | 2.48                     | 0.48              |
| 1:AA:1225:A:H2'   | 1:AA:1225:A:N3     | 2.29                     | 0.48              |
| 1:AA:1487:G:O2'   | 1:AA:1488:G:H5'    | 2.13                     | 0.48              |
| 3:AD:66:VAL:HG13  | 3:AD:70:GLN:OE1    | 2.13                     | 0.48              |
| 3:AD:201:GLU:OE1  | 4:AE:104:ILE:HG22  | 2.14                     | 0.48              |
| 13:AN:50:LEU:CD2  | 13:AN:51:PRO:HD3   | 2.41                     | 0.48              |
| 16:AQ:30:HIS:H    | 16:AQ:35:LYS:H     | 1.61                     | 0.48              |
| 23:BB:132:G:H2'   | 23:BB:133:U:C6     | 2.49                     | 0.48              |
| 23:BB:188:G:O2'   | 23:BB:189:G:H5'    | 2.14                     | 0.48              |
| 23:BB:207:A:H2'   | 23:BB:208:C:O4'    | 2.14                     | 0.48              |
| 23:BB:673:C:O2'   | 23:BB:674:G:H5'    | 2.13                     | 0.48              |
| 23:BB:942:G:O2'   | 23:BB:943:A:H5'    | 2.14                     | 0.48              |
| 23:BB:1156:A:H62  | 38:BQ:47:ARG:CD    | 2.27                     | 0.48              |
| 23:BB:1206:G:H2'  | 23:BB:1207:C:C6    | 2.49                     | 0.48              |
| 23:BB:1467:U:C4   | 23:BB:1546:G:C2    | 3.01                     | 0.48              |
| 23:BB:1583:A:H4'  | 23:BB:1585:C:N3    | 2.28                     | 0.48              |
| 23:BB:1657:U:P    | 26:BD:141:ARG:HB2  | 2.54                     | 0.48              |
| 23:BB:1791:A:H61  | 23:BB:1828:G:H1'   | 1.78                     | 0.48              |
| 23:BB:1818:U:H5'' | 25:BC:155:ARG:HG2  | 1.95                     | 0.48              |
| 23:BB:1841:U:H2'  | 23:BB:1842:G:H8    | 1.79                     | 0.48              |
| 23:BB:2149:U:O2'  | 23:BB:2150:C:H5'   | 2.13                     | 0.48              |
| 23:BB:2259:U:O2   | 23:BB:2259:U:H2'   | 2.13                     | 0.48              |
| 23:BB:2394:C:OP1  | 33:BL:63:LYS:O     | 2.30                     | 0.48              |
| 23:BB:2572:A:OP2  | 26:BD:151:THR:HA   | 2.14                     | 0.48              |
| 23:BB:2893:A:H4'  | 23:BB:2894:G:C5'   | 2.43                     | 0.48              |
| 24:BV:26:PHE:HZ   | 24:BV:47:VAL:HB    | 1.79                     | 0.48              |
| 24:BV:77:VAL:O    | 24:BV:77:VAL:HG13  | 2.14                     | 0.48              |
| 24:BV:78:GLN:HB2  | 24:BV:88:HIS:O     | 2.14                     | 0.48              |
| 25:BC:87:SER:N    | 25:BC:155:ARG:HH12 | 2.11                     | 0.48              |
| 25:BC:229:HIS:ND1 | 25:BC:230:PRO:HD2  | 2.28                     | 0.48              |
| 26:BD:1:MET:SD    | 26:BD:84:LEU:HD13  | 2.54                     | 0.48              |
| 27:BE:25:GLU:O    | 27:BE:26:ALA:C     | 2.56                     | 0.48              |
| 28:BF:59:ILE:HD11 | 28:BF:137:PHE:CG   | 2.49                     | 0.48              |
| 29:BG:18:ILE:HD13 | 29:BG:18:ILE:N     | 2.29                     | 0.48              |
| 30:BH:81:ALA:CB   | 30:BH:147:VAL:H    | 2.27                     | 0.48              |
| 31:BJ:21:THR:HA   | 31:BJ:61:LYS:HB2   | 1.95                     | 0.48              |
| 31:BJ:58:ASN:C    | 31:BJ:60:ASP:H     | 2.21                     | 0.48              |
| 33:BL:38:GLN:H    | 33:BL:41:ARG:NH1   | 2.11                     | 0.48              |
| 37:BP:93:LYS:CB   | 37:BP:96:LEU:HA    | 2.43                     | 0.48              |
| 39:BR:37:GLU:HG2  | 39:BR:62:GLU:N     | 2.19                     | 0.48              |
| 41:BT:34:VAL:HG11 | 41:BT:43:ILE:HD11  | 1.94                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:BZ:31:ASP:O     | 46:BZ:32:LEU:HB3   | 2.14                     | 0.48              |
| 50:B3:12:ARG:NH2   | 50:B3:55:GLY:HA3   | 2.28                     | 0.48              |
| 51:B4:2:LYS:HB3    | 51:B4:2:LYS:HZ2    | 1.79                     | 0.48              |
| 52:BI:58:ILE:HD12  | 52:BI:58:ILE:N     | 2.29                     | 0.48              |
| 1:CA:591:U:H2'     | 1:CA:592:G:C8      | 2.48                     | 0.48              |
| 1:CA:766:A:H2'     | 1:CA:767:A:O4'     | 2.13                     | 0.48              |
| 1:CA:1008:U:H3'    | 1:CA:1009:U:H5''   | 1.95                     | 0.48              |
| 1:CA:1020:G:N3     | 1:CA:1020:G:H2'    | 2.29                     | 0.48              |
| 1:CA:1310:G:O2'    | 1:CA:1311:A:H5'    | 2.13                     | 0.48              |
| 1:CA:1435:G:H2'    | 1:CA:1436:U:C6     | 2.49                     | 0.48              |
| 3:CD:156:ALA:O     | 3:CD:160:LEU:HD12  | 2.14                     | 0.48              |
| 4:CE:17:VAL:HA     | 4:CE:33:THR:O      | 2.13                     | 0.48              |
| 4:CE:19:ARG:O      | 4:CE:20:VAL:HB     | 2.14                     | 0.48              |
| 6:CG:112:ASP:HB2   | 6:CG:118:ARG:CG    | 2.41                     | 0.48              |
| 8:CI:40:ARG:HA     | 8:CI:44:ARG:NH1    | 2.29                     | 0.48              |
| 10:CK:121:ARG:HH21 | 21:CU:34:ARG:NE    | 2.11                     | 0.48              |
| 11:CL:75:GLU:OE2   | 11:CL:76:HIS:N     | 2.47                     | 0.48              |
| 12:CM:18:LEU:HD23  | 12:CM:24:VAL:HG21  | 1.94                     | 0.48              |
| 17:CR:20:ILE:HD12  | 17:CR:53:GLN:HE22  | 1.79                     | 0.48              |
| 20:CB:86:CYS:SG    | 20:CB:87:ASP:N     | 2.86                     | 0.48              |
| 23:DB:197:A:H62    | 23:DB:2430:A:H2'   | 1.78                     | 0.48              |
| 23:DB:810:U:N3     | 33:DL:37:GLY:HA2   | 2.29                     | 0.48              |
| 23:DB:871:U:H4'    | 34:DM:68:PHE:CE1   | 2.49                     | 0.48              |
| 23:DB:951:C:O2'    | 23:DB:952:G:H5'    | 2.14                     | 0.48              |
| 23:DB:1098:A:N3    | 52:DI:3:LYS:O      | 2.46                     | 0.48              |
| 23:DB:1666:G:O2'   | 23:DB:1667:G:H5'   | 2.13                     | 0.48              |
| 23:DB:1706:C:C2    | 23:DB:1757:A:H5'   | 2.48                     | 0.48              |
| 23:DB:1779:U:OP2   | 23:DB:1784:A:N6    | 2.46                     | 0.48              |
| 23:DB:2106:U:C2'   | 23:DB:2107:G:OP1   | 2.62                     | 0.48              |
| 23:DB:2344:U:H4'   | 23:DB:2345:G:OP1   | 2.13                     | 0.48              |
| 23:DB:2526:G:H2'   | 23:DB:2527:C:C6    | 2.48                     | 0.48              |
| 25:DC:139:THR:O    | 25:DC:191:LEU:HD12 | 2.14                     | 0.48              |
| 25:DC:267:VAL:HG12 | 25:DC:268:ARG:N    | 2.28                     | 0.48              |
| 35:DN:14:SER:HA    | 35:DN:17:ARG:HH12  | 1.79                     | 0.48              |
| 37:DP:18:SER:HB2   | 37:DP:87:ARG:NH2   | 2.28                     | 0.48              |
| 38:DQ:98:ALA:HA    | 38:DQ:105:PHE:CG   | 2.49                     | 0.48              |
| 38:DQ:113:LYS:C    | 38:DQ:115:ALA:H    | 2.21                     | 0.48              |
| 41:DT:47:VAL:HG13  | 41:DT:48:GLN:N     | 2.29                     | 0.48              |
| 43:DW:67:LYS:HE3   | 43:DW:71:LYS:H     | 1.78                     | 0.48              |
| 48:D1:24:LYS:HZ2   | 48:D1:24:LYS:CB    | 2.26                     | 0.48              |
| 50:D3:24:LYS:C     | 50:D3:26:ALA:H     | 2.22                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 50:D3:49:VAL:C    | 50:D3:51:LYS:H    | 2.22                     | 0.48              |
| 1:AA:60:A:HO2'    | 1:AA:61:G:P       | 2.36                     | 0.48              |
| 1:AA:66:A:H8      | 1:AA:66:A:O5'     | 1.97                     | 0.48              |
| 1:AA:476:U:O2'    | 1:AA:477:C:H5'    | 2.14                     | 0.48              |
| 1:AA:608:A:H2'    | 1:AA:609:A:O4'    | 2.14                     | 0.48              |
| 1:AA:840:C:C2     | 1:AA:842:U:H4'    | 2.49                     | 0.48              |
| 1:AA:1018:G:H2'   | 1:AA:1019:A:H8    | 1.77                     | 0.48              |
| 1:AA:1071:C:O2'   | 1:AA:1072:G:H5'   | 2.14                     | 0.48              |
| 2:AC:57:GLU:HB2   | 2:AC:64:ARG:CB    | 2.43                     | 0.48              |
| 2:AC:154:GLY:HA2  | 2:AC:163:ARG:O    | 2.12                     | 0.48              |
| 3:AD:37:PRO:HD2   | 3:AD:41:GLY:HA3   | 1.96                     | 0.48              |
| 3:AD:58:GLN:O     | 3:AD:62:ARG:HG2   | 2.12                     | 0.48              |
| 4:AE:89:THR:HG22  | 4:AE:90:GLY:N     | 2.29                     | 0.48              |
| 8:AI:51:LEU:HD11  | 8:AI:82:ILE:HG21  | 1.96                     | 0.48              |
| 8:AI:56:MET:CA    | 8:AI:59:LYS:HZ2   | 2.21                     | 0.48              |
| 8:AI:79:ARG:O     | 8:AI:83:THR:HG22  | 2.14                     | 0.48              |
| 11:AL:78:VAL:O    | 11:AL:102:ASP:HB2 | 2.14                     | 0.48              |
| 13:AN:33:VAL:HG23 | 13:AN:40:ARG:HH21 | 1.79                     | 0.48              |
| 21:AU:36:PHE:C    | 21:AU:40:PRO:HD3  | 2.38                     | 0.48              |
| 23:BB:545:U:H2'   | 23:BB:547:A:P     | 2.54                     | 0.48              |
| 23:BB:562:U:H2'   | 23:BB:572:A:O4'   | 2.14                     | 0.48              |
| 23:BB:633:A:H2'   | 23:BB:634:C:C5'   | 2.41                     | 0.48              |
| 23:BB:728:G:H4'   | 25:BC:12:ARG:HH22 | 1.79                     | 0.48              |
| 23:BB:839:U:O2'   | 23:BB:1191:G:H1'  | 2.14                     | 0.48              |
| 23:BB:1157:G:H2'  | 23:BB:1158:C:H6   | 1.79                     | 0.48              |
| 23:BB:1433:A:H2'  | 23:BB:1434:A:O4'  | 2.13                     | 0.48              |
| 23:BB:2059:A:N6   | 23:BB:2503:A:H2'  | 2.29                     | 0.48              |
| 23:BB:2291:U:OP1  | 23:BB:2380:C:O2'  | 2.31                     | 0.48              |
| 23:BB:2683:C:H2'  | 23:BB:2684:U:C6   | 2.49                     | 0.48              |
| 25:BC:164:VAL:HB  | 25:BC:167:ASP:OD2 | 2.13                     | 0.48              |
| 25:BC:231:HIS:ND1 | 25:BC:231:HIS:O   | 2.47                     | 0.48              |
| 29:BG:70:LEU:O    | 29:BG:74:MET:HG3  | 2.14                     | 0.48              |
| 30:BH:3:VAL:HG22  | 30:BH:21:VAL:HG21 | 1.96                     | 0.48              |
| 30:BH:11:ASN:C    | 30:BH:13:GLY:H    | 2.22                     | 0.48              |
| 31:BJ:35:ARG:NE   | 31:BJ:39:LYS:HB3  | 2.24                     | 0.48              |
| 31:BJ:46:PRO:O    | 31:BJ:47:HIS:HB2  | 2.14                     | 0.48              |
| 35:BN:9:GLN:HE21  | 35:BN:17:ARG:HH12 | 1.61                     | 0.48              |
| 36:BO:30:ARG:O    | 36:BO:31:THR:C    | 2.57                     | 0.48              |
| 38:BQ:35:PHE:HB3  | 38:BQ:39:ILE:HD12 | 1.96                     | 0.48              |
| 38:BQ:52:ARG:CZ   | 38:BQ:55:GLN:HE21 | 2.27                     | 0.48              |
| 39:BR:42:ALA:C    | 39:BR:44:GLY:N    | 2.72                     | 0.48              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:BR:51:VAL:O     | 39:BR:52:PRO:C     | 2.57                     | 0.48              |
| 39:BR:66:HIS:N     | 39:BR:98:ILE:HD13  | 2.28                     | 0.48              |
| 41:BT:74:ILE:HG22  | 41:BT:75:GLY:N     | 2.29                     | 0.48              |
| 42:BU:95:PHE:HD1   | 42:BU:96:LYS:HG2   | 1.78                     | 0.48              |
| 42:BU:96:LYS:HE2   | 42:BU:98:ASN:HB3   | 1.96                     | 0.48              |
| 43:BW:6:GLY:C      | 43:BW:8:SER:N      | 2.72                     | 0.48              |
| 45:BY:35:VAL:CG1   | 45:BY:37:ARG:HH21  | 2.27                     | 0.48              |
| 47:B0:28:SER:O     | 47:B0:36:LYS:HB2   | 2.13                     | 0.48              |
| 52:BI:17:ALA:O     | 52:BI:18:ASN:CB    | 2.62                     | 0.48              |
| 1:CA:554:A:H2'     | 1:CA:555:U:C6      | 2.49                     | 0.48              |
| 1:CA:869:G:H4'     | 1:CA:872:A:C8      | 2.49                     | 0.48              |
| 1:CA:1254:A:H2'    | 1:CA:1255:G:C8     | 2.49                     | 0.48              |
| 1:CA:1366:C:H2'    | 1:CA:1367:C:H6     | 1.77                     | 0.48              |
| 2:CC:168:ARG:HG2   | 2:CC:169:GLU:N     | 2.28                     | 0.48              |
| 4:CE:146:MET:HE2   | 4:CE:146:MET:C     | 2.38                     | 0.48              |
| 5:CF:12:PRO:HB3    | 5:CF:56:LYS:O      | 2.13                     | 0.48              |
| 5:CF:38:ARG:NH2    | 5:CF:63:ASN:ND2    | 2.59                     | 0.48              |
| 6:CG:75:LYS:HE3    | 6:CG:76:SER:O      | 2.13                     | 0.48              |
| 7:CH:88:LYS:HD3    | 7:CH:89:ASP:N      | 2.29                     | 0.48              |
| 8:CI:29:ILE:HB     | 8:CI:64:ILE:HD12   | 1.95                     | 0.48              |
| 10:CK:110:THR:HG22 | 21:CU:5:VAL:N      | 2.23                     | 0.48              |
| 11:CL:51:VAL:HG12  | 11:CL:52:CYS:N     | 2.27                     | 0.48              |
| 12:CM:102:LYS:NZ   | 12:CM:103:THR:HG23 | 2.28                     | 0.48              |
| 16:CQ:10:ARG:NE    | 16:CQ:56:ASP:O     | 2.44                     | 0.48              |
| 17:CR:47:ARG:CZ    | 17:CR:48:ALA:H     | 2.27                     | 0.48              |
| 21:CU:39:LYS:H     | 21:CU:40:PRO:CD    | 2.21                     | 0.48              |
| 22:DA:49:C:H4'     | 36:DO:68:LYS:NZ    | 2.27                     | 0.48              |
| 23:DB:150:U:H2'    | 23:DB:151:C:H6     | 1.78                     | 0.48              |
| 23:DB:963:U:H2'    | 23:DB:964:C:C6     | 2.49                     | 0.48              |
| 23:DB:1197:G:O2'   | 23:DB:1198:U:H5'   | 2.14                     | 0.48              |
| 23:DB:1213:A:C6    | 23:DB:1237:A:H1'   | 2.49                     | 0.48              |
| 23:DB:1438:U:O2'   | 23:DB:1439:A:H5'   | 2.14                     | 0.48              |
| 23:DB:1467:U:C4    | 23:DB:1546:G:C2    | 3.01                     | 0.48              |
| 23:DB:1688:U:O2    | 23:DB:1700:A:H5'   | 2.13                     | 0.48              |
| 23:DB:1819:A:OP1   | 25:DC:155:ARG:HB3  | 2.14                     | 0.48              |
| 23:DB:1821:A:H2'   | 23:DB:1822:C:H6    | 1.76                     | 0.48              |
| 23:DB:2038:G:H2'   | 23:DB:2039:U:C6    | 2.49                     | 0.48              |
| 23:DB:2261:C:OP2   | 43:DW:13:ARG:HB2   | 2.14                     | 0.48              |
| 23:DB:2466:C:O2'   | 34:DM:118:LYS:HE2  | 2.13                     | 0.48              |
| 23:DB:2773:C:H5''  | 26:DD:169:ARG:HB2  | 1.95                     | 0.48              |
| 25:DC:128:THR:HA   | 25:DC:189:ALA:O    | 2.14                     | 0.48              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:DD:121:THR:HG21 | 26:DD:143:PRO:HD3  | 1.96                     | 0.48              |
| 27:DE:134:LEU:N    | 27:DE:134:LEU:HD22 | 2.27                     | 0.48              |
| 33:DL:74:THR:O     | 33:DL:75:ALA:C     | 2.57                     | 0.48              |
| 33:DL:77:ILE:HG21  | 33:DL:92:LEU:HG    | 1.96                     | 0.48              |
| 36:DO:39:VAL:O     | 36:DO:39:VAL:HG13  | 2.13                     | 0.48              |
| 37:DP:87:ARG:HH11  | 37:DP:87:ARG:HG2   | 1.79                     | 0.48              |
| 38:DQ:55:GLN:O     | 38:DQ:58:GLN:HG3   | 2.12                     | 0.48              |
| 41:DT:63:VAL:O     | 41:DT:79:ASP:HA    | 2.14                     | 0.48              |
| 45:DY:2:LYS:CA     | 45:DY:37:ARG:HB2   | 2.44                     | 0.48              |
| 50:D3:4:LYS:HE3    | 50:D3:61:LEU:CB    | 2.44                     | 0.48              |
| 1:AA:16:A:N1       | 1:AA:919:A:H2      | 2.12                     | 0.48              |
| 1:AA:36:C:H5'      | 11:AL:119:LYS:HB3  | 1.94                     | 0.48              |
| 1:AA:110:C:H2'     | 1:AA:111:G:O4'     | 2.14                     | 0.48              |
| 1:AA:113:G:H1'     | 1:AA:354:G:H5'     | 1.96                     | 0.48              |
| 1:AA:333:U:H2'     | 1:AA:334:C:C6      | 2.49                     | 0.48              |
| 1:AA:659:U:H2'     | 1:AA:660:C:C6      | 2.49                     | 0.48              |
| 3:AD:154:VAL:HG13  | 3:AD:155:LYS:N     | 2.25                     | 0.48              |
| 12:AM:18:LEU:O     | 12:AM:21:ILE:HG13  | 2.13                     | 0.48              |
| 19:AT:59:ARG:HH11  | 19:AT:59:ARG:CB    | 2.25                     | 0.48              |
| 20:AB:71:THR:HG23  | 20:AB:93:HIS:C     | 2.39                     | 0.48              |
| 20:AB:127:LYS:HB2  | 20:AB:127:LYS:NZ   | 2.29                     | 0.48              |
| 23:BB:36:G:H4'     | 23:BB:451:U:C2     | 2.49                     | 0.48              |
| 23:BB:84:A:H3'     | 42:BU:5:ARG:HG3    | 1.96                     | 0.48              |
| 23:BB:388:G:N7     | 23:BB:390:U:H2'    | 2.28                     | 0.48              |
| 23:BB:503:A:H4'    | 23:BB:504:A:H5'    | 1.94                     | 0.48              |
| 23:BB:921:C:H2'    | 23:BB:922:C:H6     | 1.79                     | 0.48              |
| 23:BB:947:A:O2'    | 23:BB:984:A:H2     | 1.97                     | 0.48              |
| 23:BB:992:C:H1'    | 39:BR:91:GLN:CB    | 2.44                     | 0.48              |
| 23:BB:1315:C:H2'   | 23:BB:1316:U:H6    | 1.77                     | 0.48              |
| 23:BB:1537:G:H2'   | 23:BB:1538:G:O4'   | 2.14                     | 0.48              |
| 23:BB:1662:U:O2    | 23:BB:2687:U:H4'   | 2.13                     | 0.48              |
| 23:BB:2526:G:H2'   | 23:BB:2527:C:H6    | 1.79                     | 0.48              |
| 23:BB:2568:U:H2'   | 23:BB:2569:G:O4'   | 2.14                     | 0.48              |
| 23:BB:2737:G:H2'   | 23:BB:2738:A:C8    | 2.48                     | 0.48              |
| 23:BB:2845:U:H2'   | 23:BB:2846:G:C8    | 2.49                     | 0.48              |
| 24:BV:60:VAL:HG13  | 24:BV:72:VAL:O     | 2.13                     | 0.48              |
| 25:BC:64:VAL:HB    | 25:BC:65:ASP:H     | 1.42                     | 0.48              |
| 25:BC:79:ARG:NH2   | 25:BC:110:LYS:HD3  | 2.29                     | 0.48              |
| 26:BD:38:LYS:CD    | 26:BD:38:LYS:N     | 2.76                     | 0.48              |
| 26:BD:110:THR:HG22 | 26:BD:171:THR:CA   | 2.42                     | 0.48              |
| 28:BF:56:LEU:HA    | 28:BF:59:ILE:CG2   | 2.44                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:BJ:35:ARG:NH2   | 31:BJ:40:HIS:N    | 2.61                     | 0.48              |
| 32:BK:85:VAL:O     | 32:BK:87:LEU:HD23 | 2.14                     | 0.48              |
| 33:BL:27:LEU:HD12  | 33:BL:27:LEU:N    | 2.23                     | 0.48              |
| 34:BM:7:THR:HG23   | 34:BM:91:TYR:OH   | 2.14                     | 0.48              |
| 35:BN:19:ALA:C     | 35:BN:21:PHE:H    | 2.22                     | 0.48              |
| 36:BO:40:ILE:H     | 36:BO:40:ILE:CD1  | 2.27                     | 0.48              |
| 36:BO:87:ILE:CG1   | 36:BO:88:LYS:N    | 2.76                     | 0.48              |
| 37:BP:76:HIS:CD2   | 37:BP:76:HIS:N    | 2.82                     | 0.48              |
| 39:BR:1:MET:HA     | 39:BR:46:GLU:CB   | 2.43                     | 0.48              |
| 40:BS:6:LYS:CA     | 40:BS:104:THR:HA  | 2.32                     | 0.48              |
| 40:BS:31:GLN:HB3   | 40:BS:35:ILE:CG2  | 2.44                     | 0.48              |
| 46:BZ:3:LYS:CE     | 46:BZ:8:LYS:HA    | 2.41                     | 0.48              |
| 47:B0:28:SER:O     | 47:B0:29:VAL:HG12 | 2.13                     | 0.48              |
| 47:B0:32:THR:HG22  | 47:B0:32:THR:O    | 2.13                     | 0.48              |
| 52:BI:37:PHE:CZ    | 52:BI:58:ILE:HD11 | 2.49                     | 0.48              |
| 1:CA:78:A:O2'      | 1:CA:79:G:H5'     | 2.14                     | 0.48              |
| 1:CA:110:C:H2'     | 1:CA:111:G:O4'    | 2.14                     | 0.48              |
| 1:CA:627:G:H2'     | 1:CA:628:G:C8     | 2.48                     | 0.48              |
| 1:CA:708:C:H2'     | 1:CA:709:U:H6     | 1.79                     | 0.48              |
| 1:CA:737:C:H2'     | 1:CA:738:C:H6     | 1.79                     | 0.48              |
| 1:CA:1343:G:H1'    | 8:CI:122:ARG:HH12 | 1.79                     | 0.48              |
| 1:CA:1426:G:H2'    | 1:CA:1427:C:H6    | 1.79                     | 0.48              |
| 1:CA:1480:A:H2'    | 1:CA:1481:U:H6    | 1.79                     | 0.48              |
| 3:CD:64:TYR:CE2    | 3:CD:93:LEU:HD13  | 2.48                     | 0.48              |
| 9:CJ:40:ILE:CG1    | 9:CJ:73:LEU:HB3   | 2.44                     | 0.48              |
| 9:CJ:59:LYS:C      | 9:CJ:61:ALA:H     | 2.21                     | 0.48              |
| 20:CB:65:LYS:CB    | 20:CB:157:PRO:HA  | 2.43                     | 0.48              |
| 20:CB:101:THR:HG22 | 20:CB:174:GLU:CD  | 2.39                     | 0.48              |
| 22:DA:33:G:O2'     | 22:DA:34:A:H5'    | 2.14                     | 0.48              |
| 23:DB:137:U:H2'    | 23:DB:138:U:O4'   | 2.13                     | 0.48              |
| 23:DB:188:G:O2'    | 23:DB:189:G:H5'   | 2.14                     | 0.48              |
| 23:DB:234:U:C2'    | 23:DB:235:U:H5'   | 2.44                     | 0.48              |
| 23:DB:607:U:P      | 27:DE:98:LYS:HG3  | 2.54                     | 0.48              |
| 23:DB:616:A:H3'    | 23:DB:617:G:C8    | 2.44                     | 0.48              |
| 23:DB:942:G:H2'    | 23:DB:943:A:H8    | 1.79                     | 0.48              |
| 23:DB:1165:A:H2'   | 23:DB:1166:G:H8   | 1.77                     | 0.48              |
| 23:DB:1219:U:OP2   | 38:DQ:18:LYS:HE3  | 2.14                     | 0.48              |
| 23:DB:1579:A:H2'   | 23:DB:1580:A:H8   | 1.78                     | 0.48              |
| 23:DB:1903:G:OP1   | 25:DC:239:PHE:HA  | 2.13                     | 0.48              |
| 23:DB:2350:C:O2'   | 23:DB:2351:G:H5'  | 2.14                     | 0.48              |
| 23:DB:2376:A:H2    | 36:DO:117:PHE:HD2 | 1.61                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:DD:105:LYS:O   | 26:DD:177:VAL:HG12 | 2.14                     | 0.48              |
| 30:DH:8:LYS:HE2   | 30:DH:9:VAL:N      | 2.27                     | 0.48              |
| 32:DK:63:VAL:CG1  | 32:DK:103:VAL:HG12 | 2.44                     | 0.48              |
| 33:DL:51:GLU:N    | 33:DL:51:GLU:OE1   | 2.47                     | 0.48              |
| 33:DL:57:LEU:HB3  | 50:D3:54:LEU:HD22  | 1.95                     | 0.48              |
| 33:DL:90:VAL:HG12 | 33:DL:122:VAL:HG22 | 1.96                     | 0.48              |
| 37:DP:70:GLU:HG2  | 37:DP:71:ARG:HG2   | 1.96                     | 0.48              |
| 44:DX:43:LEU:HD22 | 44:DX:43:LEU:N     | 2.29                     | 0.48              |
| 46:DZ:1:MET:HE2   | 46:DZ:2:LYS:HD2    | 1.95                     | 0.48              |
| 47:D0:16:ARG:C    | 47:D0:18:HIS:H     | 2.21                     | 0.48              |
| 1:AA:434:U:O2     | 1:AA:434:U:H2'     | 2.15                     | 0.47              |
| 1:AA:634:C:O2'    | 1:AA:635:A:H5'     | 2.14                     | 0.47              |
| 1:AA:782:A:H2'    | 1:AA:783:C:O4'     | 2.14                     | 0.47              |
| 1:AA:1356:G:H2'   | 1:AA:1357:A:C8     | 2.48                     | 0.47              |
| 3:AD:100:VAL:HG13 | 3:AD:104:MET:HE3   | 1.94                     | 0.47              |
| 12:AM:89:ARG:NH1  | 12:AM:94:LEU:HD13  | 2.29                     | 0.47              |
| 17:AR:23:LYS:C    | 17:AR:25:ILE:H     | 2.22                     | 0.47              |
| 19:AT:60:GLN:C    | 19:AT:62:ALA:H     | 2.22                     | 0.47              |
| 20:AB:27:LYS:HB3  | 20:AB:28:PRO:HD3   | 1.96                     | 0.47              |
| 20:AB:174:GLU:O   | 20:AB:178:LEU:HD23 | 2.14                     | 0.47              |
| 23:BB:209:C:H2'   | 23:BB:210:C:C6     | 2.48                     | 0.47              |
| 23:BB:256:A:O2'   | 23:BB:257:C:H5'    | 2.14                     | 0.47              |
| 23:BB:753:A:H2'   | 23:BB:754:U:H6     | 1.78                     | 0.47              |
| 23:BB:852:U:H5'   | 45:BY:45:GLY:HA3   | 1.96                     | 0.47              |
| 23:BB:1299:G:H4'  | 23:BB:1301:A:C1'   | 2.42                     | 0.47              |
| 23:BB:1534:U:O2'  | 23:BB:1535:A:H8    | 1.93                     | 0.47              |
| 23:BB:1681:G:N3   | 23:BB:1762:A:H2'   | 2.29                     | 0.47              |
| 23:BB:1957:C:H2'  | 23:BB:1958:C:C6    | 2.48                     | 0.47              |
| 23:BB:2144:G:H2'  | 23:BB:2146:C:OP2   | 2.14                     | 0.47              |
| 23:BB:2462:C:H2'  | 23:BB:2463:C:C6    | 2.49                     | 0.47              |
| 23:BB:2800:A:H2'  | 23:BB:2801:G:C4'   | 2.43                     | 0.47              |
| 23:BB:2815:C:H2'  | 23:BB:2816:G:H8    | 1.79                     | 0.47              |
| 23:BB:2864:G:H2'  | 23:BB:2865:U:C6    | 2.49                     | 0.47              |
| 26:BD:8:LYS:O     | 26:BD:9:VAL:HG22   | 2.13                     | 0.47              |
| 26:BD:16:THR:CG2  | 26:BD:17:GLU:H     | 2.14                     | 0.47              |
| 26:BD:26:VAL:HG23 | 26:BD:187:LEU:HB3  | 1.96                     | 0.47              |
| 28:BF:2:LYS:HB2   | 28:BF:100:GLU:HG2  | 1.96                     | 0.47              |
| 29:BG:42:VAL:HG12 | 29:BG:51:PHE:CD1   | 2.49                     | 0.47              |
| 29:BG:126:THR:CG2 | 29:BG:128:THR:HG23 | 2.44                     | 0.47              |
| 31:BJ:125:TYR:HE2 | 31:BJ:134:ALA:HB2  | 1.78                     | 0.47              |
| 32:BK:63:VAL:CG1  | 32:BK:103:VAL:HA   | 2.44                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:BM:96:ILE:CG2  | 34:BM:97:GLN:H     | 2.17                     | 0.47              |
| 35:BN:118:ARG:NH1 | 47:B0:50:GLY:HA3   | 2.29                     | 0.47              |
| 37:BP:81:ASP:O    | 37:BP:83:ILE:N     | 2.46                     | 0.47              |
| 43:BW:40:ARG:HB2  | 43:BW:41:GLY:H     | 1.58                     | 0.47              |
| 43:BW:44:PHE:CE2  | 43:BW:80:SER:HA    | 2.49                     | 0.47              |
| 46:BZ:4:ASP:O     | 46:BZ:5:ILE:C      | 2.57                     | 0.47              |
| 47:B0:30:ASP:CG   | 47:B0:31:LYS:H     | 2.22                     | 0.47              |
| 51:B4:9:LYS:O     | 51:B4:10:LEU:HB3   | 2.14                     | 0.47              |
| 1:CA:836:G:H2'    | 1:CA:837:U:H6      | 1.79                     | 0.47              |
| 1:CA:911:U:H2'    | 1:CA:912:C:C6      | 2.49                     | 0.47              |
| 1:CA:921:U:H2'    | 1:CA:922:G:O4'     | 2.13                     | 0.47              |
| 1:CA:954:G:H2'    | 1:CA:955:U:H6      | 1.79                     | 0.47              |
| 1:CA:1277:C:HO2'  | 1:CA:1279:G:H1'    | 1.79                     | 0.47              |
| 1:CA:1361:G:C2'   | 1:CA:1362:A:H5''   | 2.43                     | 0.47              |
| 2:CC:140:ALA:HB2  | 2:CC:148:ILE:HD12  | 1.96                     | 0.47              |
| 2:CC:146:LYS:HD3  | 2:CC:203:LYS:O     | 2.14                     | 0.47              |
| 3:CD:170:LEU:O    | 3:CD:170:LEU:HD12  | 2.14                     | 0.47              |
| 8:CI:29:ILE:HD13  | 8:CI:37:TYR:CD2    | 2.49                     | 0.47              |
| 14:CO:25:GLU:HA   | 14:CO:80:LEU:HD12  | 1.96                     | 0.47              |
| 18:CS:43:MET:CB   | 18:CS:61:VAL:HG11  | 2.44                     | 0.47              |
| 20:CB:68:PHE:HA   | 20:CB:161:PHE:O    | 2.14                     | 0.47              |
| 23:DB:396:G:H2'   | 23:DB:397:U:C6     | 2.49                     | 0.47              |
| 23:DB:582:A:H2'   | 23:DB:583:G:C8     | 2.47                     | 0.47              |
| 23:DB:636:G:OP2   | 33:DL:126:ARG:NH2  | 2.47                     | 0.47              |
| 23:DB:704:G:O2'   | 23:DB:726:G:N2     | 2.46                     | 0.47              |
| 23:DB:853:C:H2'   | 23:DB:854:C:H6     | 1.78                     | 0.47              |
| 23:DB:871:U:H2'   | 23:DB:872:U:C6     | 2.49                     | 0.47              |
| 23:DB:1133:A:N6   | 23:DB:2025:C:O2'   | 2.46                     | 0.47              |
| 23:DB:1531:C:H2'  | 23:DB:1532:A:H8    | 1.75                     | 0.47              |
| 23:DB:1658:C:OP1  | 26:DD:136:ASN:ND2  | 2.47                     | 0.47              |
| 23:DB:1681:G:N3   | 23:DB:1762:A:H2'   | 2.29                     | 0.47              |
| 23:DB:1685:C:H2'  | 23:DB:1686:C:H6    | 1.78                     | 0.47              |
| 23:DB:2143:C:H2'  | 23:DB:2144:G:C4'   | 2.43                     | 0.47              |
| 23:DB:2220:U:H2'  | 23:DB:2221:G:C8    | 2.48                     | 0.47              |
| 23:DB:2527:C:OP1  | 51:D4:34:LYS:HE2   | 2.14                     | 0.47              |
| 23:DB:2593:U:O2'  | 23:DB:2594:C:H5'   | 2.13                     | 0.47              |
| 23:DB:2683:C:H2'  | 23:DB:2684:U:C6    | 2.49                     | 0.47              |
| 23:DB:2795:C:H6   | 23:DB:2795:C:O5'   | 1.96                     | 0.47              |
| 26:DD:24:VAL:HG21 | 26:DD:193:VAL:CG1  | 2.44                     | 0.47              |
| 26:DD:33:ARG:C    | 26:DD:35:THR:H     | 2.22                     | 0.47              |
| 26:DD:148:GLN:HB3 | 26:DD:151:THR:HG21 | 1.96                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DE:169:VAL:HG22 | 27:DE:170:ARG:N    | 2.28                     | 0.47              |
| 30:DH:97:ARG:HG2   | 30:DH:97:ARG:H     | 1.38                     | 0.47              |
| 31:DJ:114:LEU:HG   | 31:DJ:118:MET:CE   | 2.43                     | 0.47              |
| 32:DK:18:ARG:HB2   | 32:DK:45:GLU:CG    | 2.44                     | 0.47              |
| 32:DK:63:VAL:HG22  | 32:DK:115:ILE:HD11 | 1.95                     | 0.47              |
| 32:DK:77:ILE:HD11  | 32:DK:105:ARG:HH12 | 1.77                     | 0.47              |
| 33:DL:31:GLY:HA2   | 33:DL:36:LYS:HG2   | 1.96                     | 0.47              |
| 33:DL:140:GLY:O    | 33:DL:142:ILE:N    | 2.47                     | 0.47              |
| 36:DO:10:ARG:HG3   | 36:DO:96:GLY:H     | 1.77                     | 0.47              |
| 36:DO:25:ARG:NE    | 36:DO:94:ARG:HH12  | 2.06                     | 0.47              |
| 44:DX:51:ALA:O     | 44:DX:53:VAL:HG12  | 2.14                     | 0.47              |
| 45:DY:13:ILE:H     | 45:DY:13:ILE:HD13  | 1.79                     | 0.47              |
| 47:D0:23:ALA:C     | 47:D0:25:THR:H     | 2.21                     | 0.47              |
| 1:AA:152:A:N6      | 1:AA:170:U:C2      | 2.83                     | 0.47              |
| 1:AA:197:A:H4'     | 1:AA:198:G:O5'     | 2.15                     | 0.47              |
| 1:AA:470:C:H2'     | 1:AA:471:U:H6      | 1.79                     | 0.47              |
| 1:AA:737:C:H2'     | 1:AA:738:C:H6      | 1.79                     | 0.47              |
| 1:AA:1126:U:O2'    | 1:AA:1127:G:H5'    | 2.14                     | 0.47              |
| 1:AA:1198:G:H2'    | 1:AA:1199:U:C6     | 2.49                     | 0.47              |
| 1:AA:1221:G:OP1    | 1:AA:1320:C:N4     | 2.47                     | 0.47              |
| 1:AA:1225:A:H5'    | 12:AM:101:THR:HG23 | 1.96                     | 0.47              |
| 3:AD:67:LEU:HD22   | 3:AD:67:LEU:N      | 2.29                     | 0.47              |
| 4:AE:132:PRO:HA    | 4:AE:135:VAL:HG22  | 1.95                     | 0.47              |
| 4:AE:134:ASN:O     | 4:AE:137:ARG:HG2   | 2.13                     | 0.47              |
| 5:AF:18:VAL:HG11   | 5:AF:58:HIS:CE1    | 2.49                     | 0.47              |
| 5:AF:35:LYS:HD2    | 5:AF:65:GLU:OE2    | 2.14                     | 0.47              |
| 6:AG:102:TRP:O     | 6:AG:106:ALA:HB3   | 2.14                     | 0.47              |
| 13:AN:27:LYS:HE2   | 13:AN:48:GLN:NE2   | 2.28                     | 0.47              |
| 20:AB:10:LYS:C     | 20:AB:12:GLY:H     | 2.22                     | 0.47              |
| 20:AB:116:LEU:HB3  | 20:AB:140:LEU:CD2  | 2.44                     | 0.47              |
| 20:AB:128:LEU:CG   | 20:AB:132:GLU:HG2  | 2.44                     | 0.47              |
| 20:AB:128:LEU:HD13 | 20:AB:129:THR:H    | 1.79                     | 0.47              |
| 20:AB:209:VAL:HG23 | 20:AB:210:THR:H    | 1.77                     | 0.47              |
| 23:BB:233:A:H61    | 23:BB:428:A:N6     | 2.12                     | 0.47              |
| 23:BB:284:U:H2'    | 23:BB:285:G:C8     | 2.48                     | 0.47              |
| 23:BB:863:A:H2'    | 23:BB:864:G:C8     | 2.49                     | 0.47              |
| 23:BB:946:C:H2'    | 23:BB:947:A:C8     | 2.49                     | 0.47              |
| 23:BB:1358:G:N2    | 23:BB:1372:U:C5    | 2.82                     | 0.47              |
| 23:BB:1427:A:H4'   | 23:BB:1428:C:O4'   | 2.14                     | 0.47              |
| 23:BB:1585:C:H2'   | 23:BB:1586:A:O4'   | 2.14                     | 0.47              |
| 23:BB:2087:G:H2'   | 23:BB:2088:A:C8    | 2.49                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:2144:G:C4    | 23:BB:2146:C:H5'   | 2.49                     | 0.47              |
| 25:BC:131:MET:O    | 25:BC:134:ILE:HB   | 2.14                     | 0.47              |
| 25:BC:141:HIS:O    | 25:BC:153:LEU:HD21 | 2.14                     | 0.47              |
| 28:BF:33:ILE:HG22  | 28:BF:155:ILE:HG12 | 1.95                     | 0.47              |
| 28:BF:177:ARG:HG2  | 28:BF:178:LYS:N    | 2.28                     | 0.47              |
| 29:BG:5:LYS:NZ     | 29:BG:69:ALA:HB2   | 2.29                     | 0.47              |
| 29:BG:10:VAL:O     | 29:BG:10:VAL:HG13  | 2.13                     | 0.47              |
| 29:BG:99:GLY:C     | 29:BG:101:VAL:H    | 2.22                     | 0.47              |
| 30:BH:141:LYS:HD3  | 30:BH:141:LYS:N    | 2.29                     | 0.47              |
| 32:BK:113:MET:HE1  | 32:BK:116:ILE:CD1  | 2.44                     | 0.47              |
| 33:BL:39:LYS:HB2   | 33:BL:46:VAL:HG22  | 1.95                     | 0.47              |
| 33:BL:90:VAL:HG12  | 33:BL:121:THR:O    | 2.14                     | 0.47              |
| 34:BM:33:LEU:HB2   | 34:BM:101:VAL:HG22 | 1.96                     | 0.47              |
| 34:BM:80:VAL:O     | 34:BM:81:ARG:HB3   | 2.14                     | 0.47              |
| 37:BP:28:LYS:C     | 37:BP:44:GLY:HA3   | 2.39                     | 0.47              |
| 37:BP:112:ARG:HH11 | 37:BP:112:ARG:H    | 1.60                     | 0.47              |
| 39:BR:18:GLN:N     | 39:BR:18:GLN:OE1   | 2.47                     | 0.47              |
| 41:BT:60:THR:HG22  | 41:BT:83:ALA:CB    | 2.44                     | 0.47              |
| 41:BT:93:LEU:H     | 41:BT:93:LEU:CD2   | 2.25                     | 0.47              |
| 43:BW:46:ALA:HA    | 43:BW:57:THR:OG1   | 2.14                     | 0.47              |
| 52:BI:91:LYS:HG3   | 52:BI:91:LYS:O     | 2.13                     | 0.47              |
| 1:CA:370:C:H2'     | 1:CA:371:A:H8      | 1.77                     | 0.47              |
| 1:CA:413:G:H5'     | 1:CA:414:A:OP1     | 2.14                     | 0.47              |
| 1:CA:500:G:C5'     | 11:CL:120:ARG:HH21 | 2.28                     | 0.47              |
| 1:CA:587:G:H4'     | 7:CH:3:GLN:HA      | 1.96                     | 0.47              |
| 1:CA:1302:C:H4'    | 1:CA:1303:C:OP1    | 2.13                     | 0.47              |
| 1:CA:1404:C:H2'    | 1:CA:1405:G:H8     | 1.80                     | 0.47              |
| 1:CA:1517:G:H1'    | 23:DB:1919:A:O3'   | 2.15                     | 0.47              |
| 2:CC:2:GLN:N       | 2:CC:2:GLN:NE2     | 2.62                     | 0.47              |
| 2:CC:23:ALA:HB3    | 2:CC:28:PHE:HD1    | 1.78                     | 0.47              |
| 2:CC:71:ARG:HG3    | 2:CC:71:ARG:O      | 2.15                     | 0.47              |
| 5:CF:6:ILE:HG23    | 5:CF:62:MET:CB     | 2.35                     | 0.47              |
| 5:CF:51:ILE:HG23   | 5:CF:51:ILE:O      | 2.14                     | 0.47              |
| 10:CK:12:ARG:HB3   | 10:CK:13:LYS:HD2   | 1.96                     | 0.47              |
| 11:CL:80:LEU:HB3   | 11:CL:97:VAL:CG2   | 2.44                     | 0.47              |
| 13:CN:73:LEU:O     | 13:CN:74:ARG:C     | 2.57                     | 0.47              |
| 14:CO:81:ILE:HD12  | 14:CO:87:ARG:HB2   | 1.96                     | 0.47              |
| 20:CB:80:LYS:HA    | 20:CB:90:PHE:CZ    | 2.50                     | 0.47              |
| 22:DA:47:C:H5'     | 36:DO:97:PHE:HZ    | 1.77                     | 0.47              |
| 23:DB:16:C:O3'     | 47:D0:10:SER:HA    | 2.14                     | 0.47              |
| 23:DB:137:U:H2'    | 23:DB:138:U:C5'    | 2.45                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:298:G:C2     | 23:DB:339:U:C5     | 3.02                     | 0.47              |
| 23:DB:336:C:H5''   | 42:DU:3:LYS:HZ1    | 1.80                     | 0.47              |
| 23:DB:356:G:H2'    | 23:DB:357:C:C6     | 2.50                     | 0.47              |
| 23:DB:460:A:H2'    | 23:DB:461:C:O4'    | 2.14                     | 0.47              |
| 23:DB:491:G:H2'    | 23:DB:492:A:O4'    | 2.14                     | 0.47              |
| 23:DB:543:G:C5     | 23:DB:544:C:H1'    | 2.49                     | 0.47              |
| 23:DB:544:C:O5'    | 23:DB:545:U:OP1    | 2.32                     | 0.47              |
| 23:DB:664:G:O2'    | 23:DB:665:U:H5'    | 2.14                     | 0.47              |
| 23:DB:806:C:H2'    | 23:DB:807:U:C6     | 2.49                     | 0.47              |
| 23:DB:844:A:C2     | 23:DB:845:A:C6     | 3.02                     | 0.47              |
| 23:DB:956:G:H4'    | 34:DM:81:ARG:HH21  | 1.79                     | 0.47              |
| 23:DB:1213:A:N6    | 23:DB:1236:G:H1'   | 2.29                     | 0.47              |
| 23:DB:1358:G:N2    | 23:DB:1372:U:C5    | 2.82                     | 0.47              |
| 23:DB:1433:A:H2'   | 23:DB:1434:A:O4'   | 2.13                     | 0.47              |
| 23:DB:1585:C:H2'   | 23:DB:1586:A:O4'   | 2.14                     | 0.47              |
| 23:DB:1775:U:H2'   | 23:DB:1776:G:O4'   | 2.14                     | 0.47              |
| 23:DB:2207:C:H2'   | 23:DB:2208:C:C6    | 2.48                     | 0.47              |
| 23:DB:2519:U:H5'   | 23:DB:2567:G:N2    | 2.29                     | 0.47              |
| 23:DB:2526:G:H2'   | 23:DB:2527:C:H6    | 1.79                     | 0.47              |
| 23:DB:2647:U:O2'   | 23:DB:2648:G:H5'   | 2.15                     | 0.47              |
| 23:DB:2730:C:H4'   | 26:DD:174:SER:O    | 2.13                     | 0.47              |
| 23:DB:2828:G:O2'   | 23:DB:2829:A:H5'   | 2.14                     | 0.47              |
| 25:DC:123:ILE:HG12 | 25:DC:135:PRO:HD2  | 1.97                     | 0.47              |
| 26:DD:95:SER:O     | 26:DD:96:ILE:HG13  | 2.12                     | 0.47              |
| 26:DD:180:VAL:HG23 | 26:DD:181:ASP:H    | 1.78                     | 0.47              |
| 27:DE:152:GLU:CA   | 27:DE:188:MET:HE2  | 2.39                     | 0.47              |
| 29:DG:10:VAL:HG13  | 29:DG:14:VAL:HG12  | 1.96                     | 0.47              |
| 29:DG:10:VAL:HG13  | 29:DG:14:VAL:CG1   | 2.44                     | 0.47              |
| 30:DH:135:HIS:HB3  | 30:DH:138:VAL:CB   | 2.44                     | 0.47              |
| 31:DJ:133:ALA:O    | 31:DJ:135:GLN:N    | 2.47                     | 0.47              |
| 33:DL:14:LYS:O     | 33:DL:15:ALA:C     | 2.57                     | 0.47              |
| 35:DN:2:ARG:NH2    | 35:DN:4:ARG:HH11   | 2.12                     | 0.47              |
| 35:DN:36:THR:HG22  | 35:DN:37:THR:H     | 1.78                     | 0.47              |
| 37:DP:79:VAL:HG23  | 37:DP:81:ASP:OD1   | 2.14                     | 0.47              |
| 38:DQ:116:LEU:N    | 38:DQ:116:LEU:HD22 | 2.28                     | 0.47              |
| 41:DT:31:VAL:HG23  | 41:DT:82:LYS:HG3   | 1.95                     | 0.47              |
| 41:DT:54:GLU:HB3   | 41:DT:91:GLN:OE1   | 2.14                     | 0.47              |
| 49:D2:12:ARG:NH2   | 49:D2:16:HIS:HB2   | 2.28                     | 0.47              |
| 1:AA:790:A:N1      | 1:AA:1497:G:H5''   | 2.29                     | 0.47              |
| 2:AC:71:ARG:O      | 2:AC:74:ILE:HG22   | 2.13                     | 0.47              |
| 2:AC:171:ARG:NH1   | 2:AC:173:PRO:HG3   | 2.29                     | 0.47              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:AD:81:LEU:CD1   | 3:AD:92:LEU:HD21   | 2.44                     | 0.47              |
| 7:AH:34:ALA:HB1   | 7:AH:109:VAL:HG21  | 1.95                     | 0.47              |
| 9:AJ:5:ARG:HB3    | 9:AJ:77:VAL:HA     | 1.96                     | 0.47              |
| 9:AJ:48:ARG:HH11  | 9:AJ:48:ARG:HG2    | 1.77                     | 0.47              |
| 9:AJ:57:VAL:HG13  | 9:AJ:58:ASN:CG     | 2.39                     | 0.47              |
| 10:AK:17:ASP:HA   | 10:AK:80:ASN:O     | 2.14                     | 0.47              |
| 15:AP:67:ILE:HD11 | 15:AP:72:ALA:HA    | 1.95                     | 0.47              |
| 16:AQ:10:ARG:NE   | 16:AQ:11:VAL:H     | 2.12                     | 0.47              |
| 16:AQ:43:LEU:HD21 | 16:AQ:72:TRP:CE2   | 2.48                     | 0.47              |
| 23:BB:346:A:H5'   | 23:BB:346:A:N3     | 2.30                     | 0.47              |
| 23:BB:812:C:H4'   | 38:BQ:12:ARG:HH22  | 1.79                     | 0.47              |
| 23:BB:835:C:H5'   | 50:B3:50:SER:HB3   | 1.95                     | 0.47              |
| 23:BB:1438:U:O2'  | 23:BB:1439:A:H5'   | 2.14                     | 0.47              |
| 23:BB:1633:G:O2'  | 23:BB:1634:A:H5''  | 2.14                     | 0.47              |
| 23:BB:2350:C:O2'  | 23:BB:2351:G:H5'   | 2.13                     | 0.47              |
| 23:BB:2893:A:H4'  | 23:BB:2894:G:H5'   | 1.96                     | 0.47              |
| 55:BB:3339:HOH:O  | 27:BE:81:GLY:HA2   | 2.14                     | 0.47              |
| 25:BC:24:HIS:ND1  | 25:BC:25:LYS:N     | 2.62                     | 0.47              |
| 25:BC:63:ILE:HG22 | 25:BC:64:VAL:N     | 2.29                     | 0.47              |
| 25:BC:156:SER:O   | 25:BC:157:ALA:C    | 2.58                     | 0.47              |
| 27:BE:147:LEU:HA  | 27:BE:166:LYS:O    | 2.13                     | 0.47              |
| 28:BF:39:VAL:O    | 28:BF:39:VAL:HG12  | 2.14                     | 0.47              |
| 29:BG:32:LEU:HD21 | 29:BG:74:MET:SD    | 2.54                     | 0.47              |
| 29:BG:42:VAL:HG12 | 29:BG:51:PHE:HD1   | 1.78                     | 0.47              |
| 29:BG:140:ILE:C   | 29:BG:140:ILE:HD12 | 2.39                     | 0.47              |
| 30:BH:6:LEU:CD2   | 30:BH:50:ARG:HD3   | 2.44                     | 0.47              |
| 41:BT:33:LYS:HE3  | 41:BT:80:TRP:NE1   | 2.29                     | 0.47              |
| 47:B0:4:GLN:O     | 47:B0:5:ASN:C      | 2.57                     | 0.47              |
| 48:B1:31:GLU:H    | 48:B1:32:LYS:NZ    | 2.12                     | 0.47              |
| 1:CA:113:G:H1'    | 1:CA:354:G:H5'     | 1.96                     | 0.47              |
| 1:CA:340:U:H2'    | 1:CA:341:C:H6      | 1.78                     | 0.47              |
| 1:CA:470:C:H2'    | 1:CA:471:U:H6      | 1.79                     | 0.47              |
| 1:CA:781:A:H2'    | 1:CA:782:A:C5'     | 2.38                     | 0.47              |
| 1:CA:803:G:H2'    | 1:CA:804:U:C6      | 2.49                     | 0.47              |
| 1:CA:893:C:H2'    | 1:CA:894:G:C8      | 2.49                     | 0.47              |
| 1:CA:1527:U:OP2   | 21:CU:38:GLU:HG3   | 2.15                     | 0.47              |
| 2:CC:123:LEU:HD23 | 2:CC:195:ILE:HD12  | 1.96                     | 0.47              |
| 3:CD:21:LYS:C     | 3:CD:23:GLY:H      | 2.22                     | 0.47              |
| 3:CD:121:ALA:C    | 3:CD:145:ARG:HG3   | 2.39                     | 0.47              |
| 4:CE:89:THR:HG23  | 4:CE:90:GLY:N      | 2.29                     | 0.47              |
| 6:CG:94:ARG:HG2   | 6:CG:98:LEU:HD11   | 1.95                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:CL:23:LEU:C     | 11:CL:25:ALA:N     | 2.72                     | 0.47              |
| 11:CL:82:ARG:HH11  | 11:CL:82:ARG:HG2   | 1.79                     | 0.47              |
| 16:CQ:58:VAL:HB    | 16:CQ:74:LEU:CD2   | 2.43                     | 0.47              |
| 18:CS:39:ILE:CG2   | 18:CS:66:VAL:HA    | 2.45                     | 0.47              |
| 19:CT:54:GLN:N     | 19:CT:55:PRO:HD2   | 2.30                     | 0.47              |
| 20:CB:95:TRP:CH2   | 20:CB:99:MET:HB2   | 2.49                     | 0.47              |
| 23:DB:263:G:H2'    | 23:DB:264:C:O4'    | 2.14                     | 0.47              |
| 23:DB:851:C:O2'    | 23:DB:852:U:H5'    | 2.14                     | 0.47              |
| 23:DB:1027:A:H2    | 23:DB:2488:G:H4'   | 1.79                     | 0.47              |
| 23:DB:1515:A:H5'   | 23:DB:1557:C:C5'   | 2.44                     | 0.47              |
| 23:DB:1567:G:H5''  | 25:DC:84:PRO:HG3   | 1.96                     | 0.47              |
| 23:DB:1599:U:H2'   | 23:DB:1600:C:C6    | 2.48                     | 0.47              |
| 23:DB:1666:G:OP1   | 32:DK:66:LYS:HD2   | 2.14                     | 0.47              |
| 23:DB:1957:C:H2'   | 23:DB:1958:C:C6    | 2.49                     | 0.47              |
| 23:DB:2286:G:C8    | 23:DB:2286:G:H5'   | 2.49                     | 0.47              |
| 23:DB:2845:U:H2'   | 23:DB:2846:G:C8    | 2.49                     | 0.47              |
| 25:DC:12:ARG:HB2   | 25:DC:20:ASN:HA    | 1.96                     | 0.47              |
| 25:DC:42:ARG:CA    | 25:DC:42:ARG:HE    | 2.27                     | 0.47              |
| 25:DC:162:GLN:HE21 | 25:DC:174:ARG:NH2  | 2.12                     | 0.47              |
| 25:DC:266:ILE:HD11 | 25:DC:268:ARG:HH22 | 1.79                     | 0.47              |
| 26:DD:11:MET:O     | 26:DD:23:PRO:HD2   | 2.15                     | 0.47              |
| 28:DF:163:GLU:HG2  | 28:DF:166:ARG:NH1  | 2.28                     | 0.47              |
| 30:DH:3:VAL:CG1    | 30:DH:37:VAL:HG11  | 2.44                     | 0.47              |
| 30:DH:51:ARG:HG2   | 30:DH:51:ARG:NH1   | 2.27                     | 0.47              |
| 33:DL:39:LYS:NZ    | 33:DL:39:LYS:CA    | 2.76                     | 0.47              |
| 34:DM:57:VAL:CG1   | 34:DM:58:LYS:H     | 2.12                     | 0.47              |
| 50:D3:48:MET:HE3   | 50:D3:49:VAL:N     | 2.25                     | 0.47              |
| 1:AA:878:A:H1'     | 7:AH:3:GLN:HE22    | 1.79                     | 0.47              |
| 1:AA:1469:C:H2'    | 1:AA:1470:U:O4'    | 2.15                     | 0.47              |
| 1:AA:1504:G:H4'    | 1:AA:1505:G:N9     | 2.29                     | 0.47              |
| 2:AC:40:GLN:HE22   | 2:AC:44:LYS:HD2    | 1.80                     | 0.47              |
| 2:AC:111:ASP:OD2   | 2:AC:114:LEU:HG    | 2.14                     | 0.47              |
| 5:AF:63:ASN:HD22   | 5:AF:96:VAL:HB     | 1.79                     | 0.47              |
| 6:AG:117:LEU:HD13  | 6:AG:117:LEU:C     | 2.39                     | 0.47              |
| 12:AM:89:ARG:HH11  | 12:AM:94:LEU:HD13  | 1.79                     | 0.47              |
| 12:AM:109:LYS:HG3  | 12:AM:110:GLY:H    | 1.78                     | 0.47              |
| 13:AN:84:ARG:HH11  | 13:AN:84:ARG:HG3   | 1.80                     | 0.47              |
| 15:AP:42:ILE:CB    | 15:AP:46:LYS:HD2   | 2.29                     | 0.47              |
| 18:AS:40:PHE:HB3   | 18:AS:43:MET:HG3   | 1.96                     | 0.47              |
| 20:AB:95:TRP:CZ3   | 20:AB:171:ALA:HA   | 2.49                     | 0.47              |
| 20:AB:113:LEU:O    | 20:AB:113:LEU:HD23 | 2.15                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:160:A:H2'    | 23:BB:161:A:C8     | 2.49                     | 0.47              |
| 23:BB:338:G:N2     | 23:BB:339:U:H1'    | 2.29                     | 0.47              |
| 23:BB:399:U:OP2    | 46:BZ:49:ARG:NH1   | 2.48                     | 0.47              |
| 23:BB:640:C:H1'    | 50:B3:44:ARG:HH21  | 1.80                     | 0.47              |
| 23:BB:675:A:OP1    | 27:BE:58:LYS:HG2   | 2.14                     | 0.47              |
| 23:BB:702:U:H2'    | 23:BB:703:U:C6     | 2.49                     | 0.47              |
| 23:BB:806:C:H2'    | 23:BB:807:U:C6     | 2.50                     | 0.47              |
| 23:BB:1131:G:H1'   | 31:BJ:85:LYS:NZ    | 2.28                     | 0.47              |
| 23:BB:1239:G:H2'   | 23:BB:1240:U:C6    | 2.50                     | 0.47              |
| 23:BB:1328:A:H2'   | 23:BB:1330:C:C4    | 2.50                     | 0.47              |
| 23:BB:1847:A:H4'   | 23:BB:1848:A:H8    | 1.78                     | 0.47              |
| 23:BB:2222:C:O2'   | 23:BB:2223:G:H5'   | 2.14                     | 0.47              |
| 23:BB:2344:U:H4'   | 23:BB:2345:G:OP1   | 2.14                     | 0.47              |
| 23:BB:2393:U:O2'   | 23:BB:2394:C:H5'   | 2.15                     | 0.47              |
| 23:BB:2572:A:OP1   | 26:BD:151:THR:CG2  | 2.62                     | 0.47              |
| 23:BB:2615:U:C4    | 47:B0:2:VAL:O      | 2.68                     | 0.47              |
| 23:BB:2647:U:O2'   | 23:BB:2648:G:H5'   | 2.14                     | 0.47              |
| 23:BB:2757:A:H2'   | 23:BB:2757:A:N3    | 2.28                     | 0.47              |
| 25:BC:66:PHE:O     | 25:BC:68:ARG:N     | 2.47                     | 0.47              |
| 26:BD:61:THR:H     | 26:BD:62:LYS:HE3   | 1.78                     | 0.47              |
| 26:BD:129:THR:O    | 26:BD:130:GLN:CB   | 2.62                     | 0.47              |
| 27:BE:118:LEU:HD11 | 27:BE:187:VAL:HG12 | 1.96                     | 0.47              |
| 27:BE:159:LEU:O    | 27:BE:159:LEU:HD23 | 2.15                     | 0.47              |
| 30:BH:132:PHE:CB   | 30:BH:140:ALA:HB3  | 2.44                     | 0.47              |
| 31:BJ:46:PRO:O     | 31:BJ:48:VAL:N     | 2.43                     | 0.47              |
| 31:BJ:113:PRO:O    | 31:BJ:115:GLY:N    | 2.44                     | 0.47              |
| 33:BL:25:SER:HB3   | 33:BL:27:LEU:HG    | 1.97                     | 0.47              |
| 33:BL:55:MET:N     | 33:BL:56:PRO:CD    | 2.78                     | 0.47              |
| 33:BL:61:LEU:O     | 33:BL:62:PRO:O     | 2.32                     | 0.47              |
| 35:BN:44:LEU:HD23  | 35:BN:113:ILE:CG1  | 2.37                     | 0.47              |
| 35:BN:106:ASP:O    | 35:BN:108:ALA:N    | 2.47                     | 0.47              |
| 40:BS:31:GLN:C     | 40:BS:33:LEU:N     | 2.71                     | 0.47              |
| 41:BT:40:LYS:HE3   | 41:BT:59:ASN:HA    | 1.96                     | 0.47              |
| 44:BX:1:MET:HE3    | 44:BX:1:MET:H3     | 1.79                     | 0.47              |
| 1:CA:36:C:O2'      | 1:CA:37:U:H5'      | 2.15                     | 0.47              |
| 1:CA:719:C:O2'     | 17:CR:37:LYS:HD3   | 2.15                     | 0.47              |
| 1:CA:954:G:H2'     | 1:CA:955:U:C6      | 2.50                     | 0.47              |
| 1:CA:1060:U:OP1    | 9:CJ:53:ILE:HD11   | 2.15                     | 0.47              |
| 1:CA:1524:C:H2'    | 1:CA:1525:G:H8     | 1.78                     | 0.47              |
| 2:CC:155:ARG:NH2   | 2:CC:160:GLU:HA    | 2.29                     | 0.47              |
| 3:CD:15:GLY:HA2    | 3:CD:34:GLU:HB2    | 1.97                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:CD:171:GLU:HG3   | 3:CD:182:LYS:CG   | 2.45                     | 0.47              |
| 4:CE:114:LEU:HB3   | 4:CE:119:VAL:HB   | 1.96                     | 0.47              |
| 8:CI:7:GLY:HA3     | 8:CI:81:GLY:O     | 2.14                     | 0.47              |
| 9:CJ:40:ILE:HD11   | 9:CJ:73:LEU:HB3   | 1.97                     | 0.47              |
| 9:CJ:51:VAL:O      | 9:CJ:62:ARG:HA    | 2.14                     | 0.47              |
| 14:CO:26:VAL:HG12  | 14:CO:30:LEU:HD12 | 1.96                     | 0.47              |
| 16:CQ:8:GLN:HA     | 16:CQ:59:GLU:HA   | 1.96                     | 0.47              |
| 16:CQ:13:SER:CB    | 16:CQ:21:VAL:HB   | 2.41                     | 0.47              |
| 17:CR:25:ILE:HD12  | 17:CR:25:ILE:O    | 2.15                     | 0.47              |
| 23:DB:52:A:C5      | 23:DB:118:A:C2    | 3.02                     | 0.47              |
| 23:DB:545:U:H2'    | 23:DB:547:A:OP1   | 2.15                     | 0.47              |
| 23:DB:825:A:H2'    | 23:DB:826:U:O4'   | 2.14                     | 0.47              |
| 23:DB:832:U:H2'    | 23:DB:833:A:C8    | 2.49                     | 0.47              |
| 23:DB:1561:C:H2'   | 23:DB:1562:U:C6   | 2.49                     | 0.47              |
| 23:DB:1814:G:C5'   | 25:DC:51:ARG:HG2  | 2.44                     | 0.47              |
| 23:DB:2052:A:H5'   | 26:DD:146:ILE:O   | 2.14                     | 0.47              |
| 23:DB:2383:G:N7    | 50:D3:35:LYS:HD3  | 2.30                     | 0.47              |
| 23:DB:2868:A:H2'   | 23:DB:2869:G:H8   | 1.78                     | 0.47              |
| 25:DC:61:TYR:CE1   | 25:DC:63:ILE:HD11 | 2.49                     | 0.47              |
| 26:DD:35:THR:HB    | 26:DD:48:ILE:CG1  | 2.44                     | 0.47              |
| 26:DD:116:LYS:N    | 26:DD:116:LYS:HD2 | 2.28                     | 0.47              |
| 27:DE:48:THR:HG23  | 27:DE:85:PHE:N    | 2.29                     | 0.47              |
| 30:DH:6:LEU:HB2    | 30:DH:35:LYS:CB   | 2.43                     | 0.47              |
| 30:DH:42:LYS:O     | 30:DH:45:GLU:HB3  | 2.14                     | 0.47              |
| 31:DJ:14:ASP:HB3   | 31:DJ:16:TYR:HD1  | 1.79                     | 0.47              |
| 32:DK:7:MET:SD     | 32:DK:20:MET:HB2  | 2.55                     | 0.47              |
| 33:DL:25:SER:C     | 33:DL:27:LEU:N    | 2.72                     | 0.47              |
| 35:DN:107:ASN:ND2  | 40:DS:40:ASN:HD22 | 2.10                     | 0.47              |
| 36:DO:15:ARG:HH12  | 43:DW:76:ARG:CD   | 2.27                     | 0.47              |
| 36:DO:86:GLY:C     | 36:DO:88:LYS:N    | 2.73                     | 0.47              |
| 37:DP:27:VAL:HG21  | 37:DP:84:SER:O    | 2.14                     | 0.47              |
| 37:DP:100:ARG:HH11 | 37:DP:100:ARG:CB  | 2.17                     | 0.47              |
| 39:DR:18:GLN:CA    | 39:DR:99:THR:HA   | 2.44                     | 0.47              |
| 40:DS:68:ASP:C     | 40:DS:69:LEU:HD22 | 2.40                     | 0.47              |
| 42:DU:22:GLY:C     | 42:DU:25:LYS:HZ1  | 2.23                     | 0.47              |
| 45:DY:50:VAL:HG12  | 45:DY:53:MET:HG2  | 1.96                     | 0.47              |
| 46:DZ:49:ARG:CZ    | 46:DZ:49:ARG:HB2  | 2.45                     | 0.47              |
| 47:D0:41:HIS:CE1   | 47:D0:42:ILE:HG22 | 2.49                     | 0.47              |
| 1:AA:49:U:O2'      | 1:AA:50:A:H2'     | 2.15                     | 0.47              |
| 1:AA:699:C:C3'     | 1:AA:700:G:H5''   | 2.44                     | 0.47              |
| 1:AA:831:A:O2'     | 1:AA:832:G:H5'    | 2.15                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:985:C:H2'    | 1:AA:986:U:C6      | 2.49                     | 0.47              |
| 1:AA:1002:G:N3    | 1:AA:1002:G:H2'    | 2.29                     | 0.47              |
| 1:AA:1014:A:C2    | 1:AA:1219:A:H1'    | 2.50                     | 0.47              |
| 1:AA:1257:A:H2'   | 1:AA:1257:A:N3     | 2.28                     | 0.47              |
| 3:AD:116:LEU:HB3  | 3:AD:122:ILE:HD11  | 1.97                     | 0.47              |
| 4:AE:84:VAL:HG22  | 4:AE:85:LYS:N      | 2.28                     | 0.47              |
| 6:AG:19:SER:HB2   | 6:AG:21:LEU:HD21   | 1.96                     | 0.47              |
| 9:AJ:37:ARG:HB2   | 9:AJ:77:VAL:HG11   | 1.97                     | 0.47              |
| 13:AN:17:ASP:HA   | 13:AN:21:ALA:HB3   | 1.95                     | 0.47              |
| 18:AS:51:HIS:HB2  | 18:AS:56:HIS:CE1   | 2.50                     | 0.47              |
| 22:BA:15:A:H1'    | 22:BA:109:A:N7     | 2.30                     | 0.47              |
| 23:BB:671:C:OP1   | 33:BL:48:ARG:NH1   | 2.48                     | 0.47              |
| 23:BB:716:A:C3'   | 23:BB:717:C:H5''   | 2.44                     | 0.47              |
| 23:BB:1175:A:H2'  | 23:BB:1176:U:H5'   | 1.95                     | 0.47              |
| 23:BB:1827:U:O2'  | 23:BB:1828:G:H5'   | 2.14                     | 0.47              |
| 23:BB:2014:A:H4'  | 40:BS:93:ALA:CB    | 2.45                     | 0.47              |
| 23:BB:2331:G:H21  | 23:BB:2336:A:H8    | 1.62                     | 0.47              |
| 23:BB:2828:G:O2'  | 23:BB:2829:A:H5'   | 2.14                     | 0.47              |
| 23:BB:2845:U:H5'' | 37:BP:54:LEU:HA    | 1.96                     | 0.47              |
| 23:BB:2880:C:O2   | 35:BN:93:GLY:HA3   | 2.14                     | 0.47              |
| 24:BV:53:LYS:CE   | 24:BV:55:GLU:HG3   | 2.45                     | 0.47              |
| 25:BC:22:GLU:HA   | 25:BC:202:ARG:NH1  | 2.29                     | 0.47              |
| 25:BC:155:ARG:HB3 | 25:BC:159:THR:HG21 | 1.95                     | 0.47              |
| 26:BD:37:VAL:HG22 | 26:BD:46:ARG:CD    | 2.44                     | 0.47              |
| 27:BE:73:ILE:HG22 | 27:BE:73:ILE:O     | 2.15                     | 0.47              |
| 28:BF:93:GLU:OE1  | 28:BF:94:ARG:N     | 2.47                     | 0.47              |
| 30:BH:96:THR:HB   | 30:BH:112:LYS:HB2  | 1.97                     | 0.47              |
| 31:BJ:12:LYS:HZ2  | 31:BJ:41:LYS:HG3   | 1.79                     | 0.47              |
| 33:BL:62:PRO:HB3  | 50:B3:24:LYS:HE2   | 1.95                     | 0.47              |
| 34:BM:116:ALA:HA  | 34:BM:119:LEU:HD23 | 1.97                     | 0.47              |
| 35:BN:33:ILE:HG22 | 35:BN:113:ILE:O    | 2.14                     | 0.47              |
| 37:BP:7:LEU:HD13  | 37:BP:7:LEU:C      | 2.39                     | 0.47              |
| 37:BP:106:ALA:O   | 37:BP:108:ARG:HD2  | 2.14                     | 0.47              |
| 40:BS:71:VAL:HG22 | 40:BS:107:VAL:CG1  | 2.32                     | 0.47              |
| 41:BT:30:ILE:CG2  | 41:BT:32:LEU:HD13  | 2.44                     | 0.47              |
| 42:BU:11:ILE:HG22 | 42:BU:12:VAL:N     | 2.30                     | 0.47              |
| 43:BW:22:VAL:HG12 | 43:BW:23:LYS:H     | 1.79                     | 0.47              |
| 45:BY:54:VAL:HG22 | 45:BY:55:LYS:N     | 2.24                     | 0.47              |
| 46:BZ:30:HIS:HB2  | 46:BZ:48:GLN:HB3   | 1.96                     | 0.47              |
| 46:BZ:50:ASP:HA   | 46:BZ:53:THR:CG2   | 2.44                     | 0.47              |
| 48:B1:15:GLY:CA   | 48:B1:47:ILE:HD12  | 2.44                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:B1:31:GLU:O    | 48:B1:32:LYS:HB2   | 2.13                     | 0.47              |
| 48:B1:47:ILE:HG13 | 48:B1:48:TYR:H     | 1.77                     | 0.47              |
| 52:BI:48:ILE:O    | 52:BI:49:GLU:HB3   | 2.14                     | 0.47              |
| 1:CA:333:U:H2'    | 1:CA:334:C:C6      | 2.49                     | 0.47              |
| 1:CA:470:C:O2'    | 1:CA:471:U:H5'     | 2.14                     | 0.47              |
| 1:CA:563:A:H2'    | 1:CA:567:G:C8      | 2.50                     | 0.47              |
| 1:CA:946:A:H2'    | 1:CA:947:G:H8      | 1.73                     | 0.47              |
| 1:CA:987:G:H2'    | 1:CA:988:G:H8      | 1.79                     | 0.47              |
| 1:CA:1086:U:H3    | 1:CA:1099:G:N2     | 2.03                     | 0.47              |
| 2:CC:37:LYS:O     | 2:CC:40:GLN:HG2    | 2.14                     | 0.47              |
| 2:CC:52:SER:HB3   | 2:CC:114:LEU:HD11  | 1.95                     | 0.47              |
| 4:CE:67:ARG:HH11  | 4:CE:67:ARG:CB     | 2.26                     | 0.47              |
| 8:CI:74:GLN:O     | 8:CI:78:ILE:HG13   | 2.14                     | 0.47              |
| 9:CJ:91:ASP:C     | 9:CJ:92:LEU:HD23   | 2.40                     | 0.47              |
| 11:CL:86:VAL:CG1  | 11:CL:89:LEU:HD23  | 2.44                     | 0.47              |
| 11:CL:109:ARG:C   | 11:CL:110:LYS:HD2  | 2.39                     | 0.47              |
| 14:CO:80:LEU:HD23 | 14:CO:80:LEU:C     | 2.39                     | 0.47              |
| 15:CP:52:LEU:HD11 | 15:CP:74:LEU:HD13  | 1.95                     | 0.47              |
| 20:CB:80:LYS:HA   | 20:CB:90:PHE:CE1   | 2.48                     | 0.47              |
| 20:CB:172:ILE:CD1 | 20:CB:182:VAL:HG11 | 2.45                     | 0.47              |
| 21:CU:4:LYS:O     | 21:CU:5:VAL:HG23   | 2.14                     | 0.47              |
| 22:DA:23:G:N2     | 22:DA:24:G:H1      | 2.12                     | 0.47              |
| 23:DB:82:U:H5''   | 23:DB:296:U:H5''   | 1.96                     | 0.47              |
| 23:DB:137:U:H2'   | 23:DB:138:U:H5'    | 1.96                     | 0.47              |
| 23:DB:687:C:H1'   | 49:D2:4:THR:HG22   | 1.97                     | 0.47              |
| 23:DB:1109:C:O2'  | 23:DB:1110:G:H5'   | 2.15                     | 0.47              |
| 23:DB:1116:G:H21  | 34:DM:136:MET:CE   | 2.25                     | 0.47              |
| 23:DB:1633:G:O2'  | 23:DB:1634:A:H5''  | 2.14                     | 0.47              |
| 23:DB:1657:U:OP1  | 26:DD:141:ARG:HB2  | 2.14                     | 0.47              |
| 23:DB:1818:U:H5'' | 25:DC:155:ARG:CG   | 2.44                     | 0.47              |
| 23:DB:2270:A:H4'  | 43:DW:18:LYS:CB    | 2.44                     | 0.47              |
| 23:DB:2630:G:H2'  | 23:DB:2631:G:C8    | 2.50                     | 0.47              |
| 23:DB:2680:U:C5'  | 26:DD:194:PRO:HA   | 2.44                     | 0.47              |
| 23:DB:2815:C:H2'  | 23:DB:2816:G:H8    | 1.79                     | 0.47              |
| 23:DB:2834:G:H2'  | 23:DB:2879:A:H61   | 1.78                     | 0.47              |
| 25:DC:224:MET:HG3 | 25:DC:233:GLY:CA   | 2.45                     | 0.47              |
| 26:DD:129:THR:O   | 26:DD:130:GLN:CB   | 2.62                     | 0.47              |
| 27:DE:4:VAL:HA    | 27:DE:14:VAL:CG2   | 2.45                     | 0.47              |
| 27:DE:49:ARG:C    | 27:DE:51:GLU:N     | 2.73                     | 0.47              |
| 28:DF:36:ASN:ND2  | 28:DF:87:LYS:H     | 2.12                     | 0.47              |
| 28:DF:41:GLU:H    | 28:DF:45:ASP:HB3   | 1.79                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 30:DH:93:SER:C     | 30:DH:94:ILE:HD12 | 2.39                     | 0.47              |
| 31:DJ:25:LEU:H     | 31:DJ:25:LEU:HD22 | 1.79                     | 0.47              |
| 34:DM:8:LYS:HG2    | 34:DM:9:PHE:N     | 2.28                     | 0.47              |
| 34:DM:96:ILE:HG22  | 34:DM:97:GLN:HE22 | 1.78                     | 0.47              |
| 34:DM:133:LYS:HD2  | 34:DM:134:THR:N   | 2.29                     | 0.47              |
| 38:DQ:39:ILE:C     | 38:DQ:39:ILE:HD12 | 2.40                     | 0.47              |
| 39:DR:47:VAL:HG13  | 39:DR:49:ILE:H    | 1.80                     | 0.47              |
| 39:DR:79:ARG:CD    | 39:DR:81:LYS:HG3  | 2.44                     | 0.47              |
| 40:DS:72:THR:HG23  | 40:DS:73:LYS:N    | 2.29                     | 0.47              |
| 43:DW:66:VAL:HG13  | 43:DW:67:LYS:N    | 2.24                     | 0.47              |
| 44:DX:18:LEU:H     | 44:DX:18:LEU:CD2  | 2.14                     | 0.47              |
| 46:DZ:33:ASN:HB3   | 46:DZ:46:GLY:HA2  | 1.96                     | 0.47              |
| 47:D0:36:LYS:HG3   | 47:D0:40:HIS:O    | 2.14                     | 0.47              |
| 49:D2:18:PHE:O     | 49:D2:22:MET:N    | 2.45                     | 0.47              |
| 52:DI:10:LEU:HD12  | 52:DI:10:LEU:C    | 2.39                     | 0.47              |
| 52:DI:17:ALA:O     | 52:DI:18:ASN:HB3  | 2.14                     | 0.47              |
| 1:AA:86:G:H4'      | 1:AA:86:G:OP1     | 2.13                     | 0.47              |
| 1:AA:472:U:N3      | 1:AA:473:U:C4     | 2.82                     | 0.47              |
| 1:AA:947:G:H2'     | 1:AA:948:C:C6     | 2.49                     | 0.47              |
| 1:AA:1072:G:H2'    | 1:AA:1073:U:C6    | 2.49                     | 0.47              |
| 1:AA:1110:A:C2'    | 1:AA:1111:A:H5'   | 2.44                     | 0.47              |
| 1:AA:1250:A:H4'    | 8:AI:69:GLY:N     | 2.24                     | 0.47              |
| 1:AA:1409:C:N4     | 1:AA:1491:G:N1    | 2.50                     | 0.47              |
| 4:AE:25:LYS:HE2    | 4:AE:25:LYS:C     | 2.39                     | 0.47              |
| 6:AG:47:GLU:HA     | 6:AG:47:GLU:OE1   | 2.13                     | 0.47              |
| 6:AG:112:ASP:CB    | 6:AG:118:ARG:HG2  | 2.39                     | 0.47              |
| 7:AH:111:THR:HG23  | 7:AH:114:ALA:CB   | 2.45                     | 0.47              |
| 9:AJ:39:PRO:HB3    | 9:AJ:74:VAL:HG22  | 1.96                     | 0.47              |
| 11:AL:24:GLU:HB3   | 11:AL:26:CYS:SG   | 2.54                     | 0.47              |
| 15:AP:33:ILE:HD12  | 15:AP:33:ILE:H    | 1.80                     | 0.47              |
| 15:AP:76:LYS:HD2   | 15:AP:80:LYS:HD2  | 1.97                     | 0.47              |
| 20:AB:113:LEU:HD12 | 20:AB:143:LEU:HB3 | 1.97                     | 0.47              |
| 20:AB:162:VAL:O    | 20:AB:184:ALA:HA  | 2.15                     | 0.47              |
| 21:AU:26:GLY:C     | 21:AU:28:LEU:N    | 2.72                     | 0.47              |
| 22:BA:42:C:H4'     | 28:BF:63:LYS:O    | 2.13                     | 0.47              |
| 22:BA:58:A:H2'     | 22:BA:59:A:O4'    | 2.14                     | 0.47              |
| 23:BB:142:A:O2'    | 41:BT:2:ILE:HG21  | 2.14                     | 0.47              |
| 23:BB:299:A:N6     | 23:BB:322:A:H1'   | 2.30                     | 0.47              |
| 23:BB:423:A:H5'    | 23:BB:424:G:H5'   | 1.96                     | 0.47              |
| 23:BB:832:U:H2'    | 23:BB:833:A:C8    | 2.49                     | 0.47              |
| 23:BB:859:G:O2'    | 23:BB:860:U:OP2   | 2.33                     | 0.47              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BB:956:G:C1'   | 34:BM:81:ARG:HH22 | 2.27                     | 0.47              |
| 23:BB:1113:U:OP1  | 29:BG:1:SER:C     | 2.58                     | 0.47              |
| 23:BB:1188:U:O2'  | 23:BB:1189:A:H5'  | 2.14                     | 0.47              |
| 23:BB:1882:U:O2'  | 23:BB:1883:U:H5'  | 2.14                     | 0.47              |
| 23:BB:2205:A:H2'  | 23:BB:2206:C:C6   | 2.49                     | 0.47              |
| 26:BD:41:ALA:O    | 26:BD:42:ASN:HB3  | 2.15                     | 0.47              |
| 26:BD:61:THR:C    | 26:BD:63:PRO:HD2  | 2.40                     | 0.47              |
| 28:BF:16:MET:O    | 28:BF:20:ASN:HA   | 2.14                     | 0.47              |
| 32:BK:64:ARG:HB3  | 32:BK:79:PHE:HB2  | 1.97                     | 0.47              |
| 32:BK:107:LEU:C   | 32:BK:109:SER:H   | 2.22                     | 0.47              |
| 34:BM:35:ALA:C    | 34:BM:36:VAL:HG13 | 2.40                     | 0.47              |
| 37:BP:61:ARG:O    | 37:BP:62:LYS:C    | 2.57                     | 0.47              |
| 37:BP:94:ALA:HB3  | 37:BP:99:LEU:HD13 | 1.96                     | 0.47              |
| 41:BT:26:LYS:C    | 41:BT:26:LYS:HD2  | 2.40                     | 0.47              |
| 41:BT:63:VAL:CG1  | 41:BT:80:TRP:HB2  | 2.45                     | 0.47              |
| 41:BT:64:LYS:HZ3  | 41:BT:79:ASP:HB2  | 1.80                     | 0.47              |
| 43:BW:17:ALA:O    | 43:BW:35:ILE:HA   | 2.15                     | 0.47              |
| 47:B0:7:PRO:O     | 47:B0:8:THR:C     | 2.58                     | 0.47              |
| 50:B3:24:LYS:CE   | 50:B3:29:ARG:HH22 | 2.27                     | 0.47              |
| 1:CA:152:A:N6     | 1:CA:170:U:C2     | 2.82                     | 0.47              |
| 1:CA:202:G:H1'    | 1:CA:468:A:H8     | 1.79                     | 0.47              |
| 1:CA:512:U:H2'    | 1:CA:513:C:C6     | 2.49                     | 0.47              |
| 1:CA:589:U:O2'    | 1:CA:590:U:H5'    | 2.14                     | 0.47              |
| 1:CA:792:A:H1'    | 1:CA:794:A:N7     | 2.29                     | 0.47              |
| 1:CA:1250:A:H2'   | 1:CA:1251:A:H8    | 1.79                     | 0.47              |
| 1:CA:1301:U:O2'   | 1:CA:1302:C:P     | 2.72                     | 0.47              |
| 5:CF:74:LEU:HD13  | 5:CF:74:LEU:C     | 2.39                     | 0.47              |
| 7:CH:50:VAL:O     | 7:CH:50:VAL:HG13  | 2.15                     | 0.47              |
| 10:CK:70:ALA:HB1  | 10:CK:74:LYS:CD   | 2.41                     | 0.47              |
| 11:CL:82:ARG:NH2  | 11:CL:95:HIS:ND1  | 2.63                     | 0.47              |
| 12:CM:47:LEU:HD23 | 12:CM:47:LEU:N    | 2.29                     | 0.47              |
| 15:CP:61:VAL:CA   | 15:CP:65:ALA:HB3  | 2.44                     | 0.47              |
| 19:CT:31:ILE:HD13 | 19:CT:74:HIS:CE1  | 2.49                     | 0.47              |
| 20:CB:86:CYS:C    | 20:CB:88:GLN:N    | 2.73                     | 0.47              |
| 20:CB:96:LEU:HB2  | 20:CB:99:MET:HG3  | 1.96                     | 0.47              |
| 22:DA:64:G:H2'    | 22:DA:65:U:C6     | 2.49                     | 0.47              |
| 23:DB:159:G:O2'   | 23:DB:160:A:H5''  | 2.15                     | 0.47              |
| 23:DB:580:U:O3'   | 38:DQ:30:VAL:HG13 | 2.14                     | 0.47              |
| 23:DB:928:A:O2'   | 23:DB:929:U:H5'   | 2.15                     | 0.47              |
| 23:DB:2331:G:H21  | 23:DB:2336:A:H8   | 1.62                     | 0.47              |
| 25:DC:51:ARG:O    | 25:DC:52:HIS:C    | 2.57                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:DC:86:ARG:O    | 25:DC:88:ALA:N    | 2.47                     | 0.47              |
| 26:DD:119:ALA:CB  | 26:DD:165:MET:HG2 | 2.44                     | 0.47              |
| 27:DE:21:ARG:NH1  | 27:DE:23:PHE:HB3  | 2.24                     | 0.47              |
| 27:DE:115:GLN:HG3 | 27:DE:116:ASP:N   | 2.27                     | 0.47              |
| 29:DG:124:CYS:C   | 29:DG:126:THR:H   | 2.21                     | 0.47              |
| 30:DH:12:LEU:HD23 | 30:DH:12:LEU:C    | 2.39                     | 0.47              |
| 31:DJ:44:TYR:HD1  | 31:DJ:45:THR:H    | 1.51                     | 0.47              |
| 36:DO:65:THR:HB   | 36:DO:66:GLY:H    | 1.56                     | 0.47              |
| 36:DO:92:PHE:HE2  | 36:DO:94:ARG:HE   | 1.62                     | 0.47              |
| 38:DQ:52:ARG:O    | 38:DQ:53:LYS:C    | 2.58                     | 0.47              |
| 38:DQ:72:GLY:O    | 38:DQ:73:ILE:HG22 | 2.14                     | 0.47              |
| 44:DX:49:ASP:HA   | 44:DX:52:ARG:HH12 | 1.79                     | 0.47              |
| 47:D0:12:ARG:HH21 | 47:D0:16:ARG:HG3  | 1.80                     | 0.47              |
| 47:D0:24:VAL:HG12 | 47:D0:24:VAL:O    | 2.15                     | 0.47              |
| 47:D0:29:VAL:HB   | 47:D0:34:GLY:CA   | 2.44                     | 0.47              |
| 52:DI:72:THR:HG23 | 52:DI:112:LYS:HD2 | 1.97                     | 0.47              |
| 1:AA:36:C:O2'     | 1:AA:37:U:H5'     | 2.15                     | 0.47              |
| 1:AA:202:G:H1'    | 1:AA:468:A:H8     | 1.79                     | 0.47              |
| 1:AA:470:C:O2'    | 1:AA:471:U:H5'    | 2.14                     | 0.47              |
| 1:AA:563:A:H2'    | 1:AA:567:G:C8     | 2.50                     | 0.47              |
| 1:AA:620:C:N1     | 3:AD:131:ILE:HD13 | 2.29                     | 0.47              |
| 1:AA:647:C:O2'    | 1:AA:648:A:H5'    | 2.14                     | 0.47              |
| 1:AA:792:A:H1'    | 1:AA:794:A:N7     | 2.30                     | 0.47              |
| 1:AA:824:G:O2'    | 1:AA:825:A:H5'    | 2.14                     | 0.47              |
| 1:AA:923:A:H2'    | 1:AA:924:C:H6     | 1.79                     | 0.47              |
| 1:AA:940:C:H2'    | 1:AA:941:G:H8     | 1.80                     | 0.47              |
| 1:AA:957:U:O2     | 1:AA:959:A:H8     | 1.98                     | 0.47              |
| 1:AA:963:G:H21    | 9:AJ:56:HIS:CE1   | 2.33                     | 0.47              |
| 1:AA:979:C:H2'    | 1:AA:980:C:O4'    | 2.14                     | 0.47              |
| 1:AA:1246:A:H2'   | 1:AA:1247:U:O4'   | 2.15                     | 0.47              |
| 1:AA:1348:U:H4'   | 8:AI:121:ARG:NH1  | 2.29                     | 0.47              |
| 1:AA:1423:G:H2'   | 1:AA:1424:U:O4'   | 2.14                     | 0.47              |
| 2:AC:100:ILE:O    | 2:AC:100:ILE:HG23 | 2.14                     | 0.47              |
| 2:AC:134:LYS:O    | 2:AC:138:GLN:HB2  | 2.14                     | 0.47              |
| 2:AC:166:TRP:O    | 2:AC:167:TYR:HB2  | 2.14                     | 0.47              |
| 3:AD:113:ALA:O    | 3:AD:117:VAL:HG23 | 2.15                     | 0.47              |
| 8:AI:66:VAL:HG22  | 8:AI:67:LYS:N     | 2.30                     | 0.47              |
| 10:AK:21:HIS:CE1  | 10:AK:34:THR:HG21 | 2.50                     | 0.47              |
| 10:AK:36:ARG:HG2  | 10:AK:37:GLN:N    | 2.30                     | 0.47              |
| 11:AL:30:ARG:HB3  | 11:AL:57:THR:CG2  | 2.45                     | 0.47              |
| 13:AN:60:ARG:H    | 13:AN:60:ARG:CD   | 2.15                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 14:AO:84:LEU:HD22 | 14:AO:86:LEU:HD11  | 1.96                     | 0.47              |
| 15:AP:6:LEU:HB3   | 15:AP:17:TYR:HB3   | 1.96                     | 0.47              |
| 17:AR:19:GLU:C    | 17:AR:21:ASP:H     | 2.22                     | 0.47              |
| 17:AR:64:LEU:HB2  | 17:AR:66:LEU:HG    | 1.97                     | 0.47              |
| 19:AT:70:LYS:HB2  | 19:AT:70:LYS:HZ3   | 1.78                     | 0.47              |
| 22:BA:30:C:O2     | 22:BA:30:C:H2'     | 2.15                     | 0.47              |
| 22:BA:113:C:H2'   | 22:BA:114:C:O4'    | 2.14                     | 0.47              |
| 23:BB:32:C:H2'    | 23:BB:33:C:H5''    | 1.96                     | 0.47              |
| 23:BB:41:C:O2'    | 23:BB:42:A:H5'     | 2.13                     | 0.47              |
| 23:BB:282:A:H2'   | 23:BB:283:G:H8     | 1.76                     | 0.47              |
| 23:BB:459:U:H5'   | 49:B2:41:ARG:NE    | 2.27                     | 0.47              |
| 23:BB:636:G:N7    | 33:BL:109:LYS:HE2  | 2.30                     | 0.47              |
| 23:BB:825:A:H2'   | 23:BB:826:U:O4'    | 2.14                     | 0.47              |
| 23:BB:1083:U:H1'  | 23:BB:1086:A:N6    | 2.30                     | 0.47              |
| 23:BB:1351:C:H2'  | 23:BB:1352:U:C6    | 2.50                     | 0.47              |
| 23:BB:1453:A:H62  | 35:BN:72:ASP:CG    | 2.23                     | 0.47              |
| 23:BB:1511:G:H2'  | 23:BB:1512:C:C6    | 2.50                     | 0.47              |
| 23:BB:1651:G:H4'  | 35:BN:39:PRO:HG2   | 1.97                     | 0.47              |
| 23:BB:1706:C:C2   | 23:BB:1757:A:H5'   | 2.49                     | 0.47              |
| 23:BB:1707:G:H2'  | 23:BB:1708:C:H6    | 1.79                     | 0.47              |
| 23:BB:1720:U:O2'  | 23:BB:1721:G:H5'   | 2.15                     | 0.47              |
| 23:BB:1919:A:H2'  | 23:BB:1920:C:H5'   | 1.97                     | 0.47              |
| 23:BB:2041:U:H2'  | 23:BB:2042:A:H8    | 1.73                     | 0.47              |
| 23:BB:2051:A:H5'  | 26:BD:145:SER:HB3  | 1.97                     | 0.47              |
| 23:BB:2052:A:N9   | 26:BD:155:VAL:HG23 | 2.29                     | 0.47              |
| 23:BB:2192:U:H2'  | 23:BB:2193:G:O4'   | 2.15                     | 0.47              |
| 23:BB:2616:C:H2'  | 23:BB:2617:U:H6    | 1.79                     | 0.47              |
| 23:BB:2630:G:H2'  | 23:BB:2631:G:C8    | 2.50                     | 0.47              |
| 23:BB:2756:U:H1'  | 23:BB:2757:A:H5''  | 1.97                     | 0.47              |
| 23:BB:2786:U:H4'  | 26:BD:66:GLY:HA2   | 1.96                     | 0.47              |
| 23:BB:2801:G:H2'  | 23:BB:2802:G:C8    | 2.49                     | 0.47              |
| 23:BB:2810:A:H2'  | 23:BB:2811:G:O4'   | 2.15                     | 0.47              |
| 23:BB:2862:G:H2'  | 23:BB:2863:C:H6    | 1.79                     | 0.47              |
| 24:BV:53:LYS:HD2  | 24:BV:54:ALA:N     | 2.29                     | 0.47              |
| 25:BC:38:LYS:HD3  | 25:BC:39:SER:O     | 2.14                     | 0.47              |
| 25:BC:53:ILE:HG12 | 25:BC:218:THR:HA   | 1.96                     | 0.47              |
| 25:BC:207:ALA:O   | 25:BC:208:GLY:C    | 2.57                     | 0.47              |
| 26:BD:37:VAL:HG23 | 26:BD:42:ASN:ND2   | 2.30                     | 0.47              |
| 26:BD:83:ARG:HG2  | 26:BD:84:LEU:H     | 1.80                     | 0.47              |
| 26:BD:142:VAL:C   | 26:BD:144:GLY:H    | 2.21                     | 0.47              |
| 27:BE:6:LYS:HE3   | 27:BE:118:LEU:HB2  | 1.96                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BE:74:LYS:O     | 27:BE:75:SER:C     | 2.58                     | 0.47              |
| 27:BE:143:LEU:HB3  | 27:BE:146:VAL:HG21 | 1.95                     | 0.47              |
| 27:BE:148:ILE:HG22 | 27:BE:185:LYS:H    | 1.80                     | 0.47              |
| 27:BE:148:ILE:C    | 27:BE:148:ILE:HD12 | 2.38                     | 0.47              |
| 27:BE:149:ILE:HG12 | 27:BE:186:VAL:HG22 | 1.97                     | 0.47              |
| 28:BF:35:LEU:HD12  | 28:BF:35:LEU:N     | 2.30                     | 0.47              |
| 29:BG:22:VAL:HG23  | 29:BG:33:THR:HG23  | 1.97                     | 0.47              |
| 30:BH:72:ILE:O     | 30:BH:72:ILE:HG23  | 2.14                     | 0.47              |
| 31:BJ:72:LYS:HG3   | 31:BJ:90:GLU:HG3   | 1.97                     | 0.47              |
| 33:BL:77:ILE:HA    | 33:BL:101:ILE:CD1  | 2.45                     | 0.47              |
| 33:BL:82:LEU:CD2   | 33:BL:92:LEU:HD12  | 2.44                     | 0.47              |
| 35:BN:32:GLU:HA    | 35:BN:115:LEU:HD21 | 1.95                     | 0.47              |
| 37:BP:4:ILE:O      | 37:BP:7:LEU:HB3    | 2.15                     | 0.47              |
| 37:BP:8:GLU:HA     | 37:BP:11:GLN:HG2   | 1.95                     | 0.47              |
| 40:BS:33:LEU:HB3   | 40:BS:37:THR:HB    | 1.96                     | 0.47              |
| 42:BU:8:ASP:HB3    | 42:BU:25:LYS:HE2   | 1.95                     | 0.47              |
| 42:BU:13:LEU:CD2   | 42:BU:14:THR:H     | 2.28                     | 0.47              |
| 42:BU:70:ALA:O     | 42:BU:71:ILE:C     | 2.56                     | 0.47              |
| 43:BW:11:ASN:HD22  | 43:BW:13:ARG:NH2   | 2.13                     | 0.47              |
| 43:BW:36:ILE:HD12  | 43:BW:69:GLU:CD    | 2.39                     | 0.47              |
| 45:BY:3:THR:HG21   | 45:BY:43:ILE:HB    | 1.95                     | 0.47              |
| 48:B1:31:GLU:C     | 48:B1:32:LYS:HZ2   | 2.22                     | 0.47              |
| 48:B1:33:LEU:O     | 48:B1:33:LEU:HD12  | 2.14                     | 0.47              |
| 51:B4:22:VAL:HG11  | 51:B4:36:ARG:CZ    | 2.44                     | 0.47              |
| 52:BI:92:PRO:C     | 52:BI:94:LYS:H     | 2.23                     | 0.47              |
| 1:CA:60:A:H1'      | 1:CA:61:G:O4'      | 2.14                     | 0.47              |
| 1:CA:392:C:C2      | 1:CA:393:A:C8      | 3.03                     | 0.47              |
| 1:CA:397:A:H5'     | 1:CA:398:U:OP1     | 2.13                     | 0.47              |
| 1:CA:932:C:H2'     | 1:CA:933:G:C8      | 2.50                     | 0.47              |
| 1:CA:1009:U:H1'    | 1:CA:1021:A:C6     | 2.50                     | 0.47              |
| 1:CA:1144:G:N2     | 1:CA:1146:A:H62    | 2.12                     | 0.47              |
| 1:CA:1157:A:H4'    | 1:CA:1158:C:O5'    | 2.14                     | 0.47              |
| 1:CA:1238:A:N3     | 1:CA:1241:G:H1'    | 2.30                     | 0.47              |
| 1:CA:1381:U:O2'    | 6:CG:78:ARG:HB3    | 2.15                     | 0.47              |
| 1:CA:1432:G:OP1    | 37:DP:105:LYS:HB2  | 2.15                     | 0.47              |
| 2:CC:66:THR:HG23   | 2:CC:101:ASN:HB2   | 1.97                     | 0.47              |
| 2:CC:151:GLU:HG3   | 2:CC:166:TRP:HB2   | 1.97                     | 0.47              |
| 3:CD:57:LYS:HD3    | 3:CD:58:GLN:N      | 2.29                     | 0.47              |
| 5:CF:55:HIS:ND1    | 5:CF:55:HIS:N      | 2.62                     | 0.47              |
| 6:CG:49:LEU:C      | 6:CG:51:GLN:N      | 2.73                     | 0.47              |
| 6:CG:147:ASN:C     | 6:CG:149:ALA:H     | 2.21                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:CJ:55:PRO:O     | 9:CJ:56:HIS:HB3   | 2.14                     | 0.47              |
| 12:CM:21:ILE:HB   | 12:CM:24:VAL:HG22 | 1.95                     | 0.47              |
| 19:CT:78:LEU:O    | 19:CT:82:ILE:HG23 | 2.14                     | 0.47              |
| 20:CB:86:CYS:C    | 20:CB:88:GLN:H    | 2.21                     | 0.47              |
| 20:CB:93:HIS:O    | 20:CB:94:ARG:C    | 2.57                     | 0.47              |
| 22:DA:50:A:OP1    | 36:DO:68:LYS:HB2  | 2.15                     | 0.47              |
| 22:DA:82:U:H5''   | 45:DY:16:LEU:CD1  | 2.44                     | 0.47              |
| 23:DB:8:C:O2'     | 23:DB:9:G:H5'     | 2.15                     | 0.47              |
| 23:DB:105:C:H2'   | 23:DB:106:C:C6    | 2.50                     | 0.47              |
| 23:DB:356:G:O2'   | 23:DB:357:C:H5'   | 2.14                     | 0.47              |
| 23:DB:852:U:H2'   | 23:DB:853:C:H6    | 1.79                     | 0.47              |
| 23:DB:967:U:H2'   | 23:DB:968:C:H6    | 1.78                     | 0.47              |
| 23:DB:1130:U:HO2' | 23:DB:1131:G:H8   | 1.63                     | 0.47              |
| 23:DB:1241:A:O4'  | 23:DB:1241:A:N3   | 2.48                     | 0.47              |
| 23:DB:1511:G:H2'  | 23:DB:1512:C:C6   | 2.50                     | 0.47              |
| 23:DB:1544:A:H2'  | 23:DB:1545:A:C8   | 2.49                     | 0.47              |
| 23:DB:1656:C:H5'' | 26:DD:141:ARG:HB3 | 1.96                     | 0.47              |
| 23:DB:1666:G:C2'  | 23:DB:1667:G:H5'  | 2.45                     | 0.47              |
| 23:DB:1683:U:H2'  | 23:DB:1684:G:H8   | 1.80                     | 0.47              |
| 23:DB:1824:G:H2'  | 23:DB:1825:U:C6   | 2.50                     | 0.47              |
| 23:DB:2247:A:O2'  | 23:DB:2248:C:H5'  | 2.15                     | 0.47              |
| 23:DB:2309:A:C6   | 23:DB:2310:C:N4   | 2.83                     | 0.47              |
| 23:DB:2386:A:C4'  | 43:DW:38:ARG:HB2  | 2.44                     | 0.47              |
| 23:DB:2637:U:C2'  | 23:DB:2638:G:H5'  | 2.44                     | 0.47              |
| 23:DB:2760:C:H2'  | 23:DB:2760:C:O2   | 2.13                     | 0.47              |
| 23:DB:2773:C:O2'  | 23:DB:2774:C:H5'  | 2.15                     | 0.47              |
| 23:DB:2810:A:H2'  | 23:DB:2811:G:O4'  | 2.15                     | 0.47              |
| 25:DC:42:ARG:HA   | 25:DC:42:ARG:NE   | 2.30                     | 0.47              |
| 25:DC:136:VAL:O   | 25:DC:138:SER:N   | 2.48                     | 0.47              |
| 25:DC:245:THR:O   | 25:DC:246:PRO:C   | 2.57                     | 0.47              |
| 26:DD:34:VAL:HG11 | 26:DD:50:VAL:HG23 | 1.97                     | 0.47              |
| 26:DD:46:ARG:CA   | 26:DD:82:PHE:HA   | 2.44                     | 0.47              |
| 26:DD:73:VAL:HB   | 26:DD:91:THR:CB   | 2.44                     | 0.47              |
| 26:DD:122:VAL:HA  | 26:DD:128:ARG:HD2 | 1.96                     | 0.47              |
| 27:DE:46:GLN:NE2  | 27:DE:48:THR:HB   | 2.29                     | 0.47              |
| 28:DF:34:THR:O    | 28:DF:35:LEU:HD23 | 2.15                     | 0.47              |
| 28:DF:37:MET:HB2  | 28:DF:86:CYS:SG   | 2.53                     | 0.47              |
| 29:DG:37:ASN:N    | 29:DG:40:VAL:HG21 | 2.29                     | 0.47              |
| 29:DG:57:TYR:O    | 29:DG:58:ALA:C    | 2.56                     | 0.47              |
| 31:DJ:4:PHE:CD1   | 31:DJ:5:THR:N     | 2.83                     | 0.47              |
| 31:DJ:11:VAL:HG22 | 31:DJ:11:VAL:O    | 2.13                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:DL:61:LEU:N    | 33:DL:62:PRO:CD    | 2.78                     | 0.47              |
| 34:DM:44:ARG:HB2  | 34:DM:91:TYR:HE2   | 1.80                     | 0.47              |
| 35:DN:56:LYS:HG3  | 35:DN:57:THR:N     | 2.27                     | 0.47              |
| 37:DP:7:LEU:HA    | 37:DP:10:GLU:CD    | 2.39                     | 0.47              |
| 38:DQ:47:ARG:HH12 | 38:DQ:50:ARG:CG    | 2.27                     | 0.47              |
| 38:DQ:82:LEU:HD12 | 38:DQ:112:ALA:HB2  | 1.95                     | 0.47              |
| 38:DQ:94:LEU:C    | 38:DQ:94:LEU:HD12  | 2.39                     | 0.47              |
| 39:DR:49:ILE:HG13 | 39:DR:51:VAL:CG2   | 2.42                     | 0.47              |
| 39:DR:92:TRP:HE3  | 39:DR:93:PHE:N     | 2.13                     | 0.47              |
| 41:DT:55:VAL:CG2  | 41:DT:86:THR:H     | 2.28                     | 0.47              |
| 43:DW:18:LYS:HB2  | 43:DW:18:LYS:NZ    | 2.30                     | 0.47              |
| 43:DW:42:THR:HB   | 43:DW:75:ASN:HB3   | 1.94                     | 0.47              |
| 44:DX:23:ARG:O    | 44:DX:26:PHE:HB2   | 2.14                     | 0.47              |
| 44:DX:28:LEU:HD22 | 44:DX:42:LEU:HG    | 1.95                     | 0.47              |
| 44:DX:47:ARG:HA   | 44:DX:47:ARG:HE    | 1.79                     | 0.47              |
| 45:DY:1:ALA:H2    | 45:DY:43:ILE:HB    | 1.80                     | 0.47              |
| 45:DY:6:ILE:HG12  | 45:DY:35:VAL:O     | 2.15                     | 0.47              |
| 50:D3:29:ARG:O    | 50:D3:31:ILE:N     | 2.48                     | 0.47              |
| 52:DI:12:VAL:HG13 | 52:DI:41:PHE:CE2   | 2.50                     | 0.47              |
| 1:AA:357:G:OP1    | 1:AA:367:U:H6      | 1.98                     | 0.47              |
| 1:AA:392:C:C2     | 1:AA:393:A:C8      | 3.02                     | 0.47              |
| 1:AA:408:A:H3'    | 1:AA:409:U:C6      | 2.47                     | 0.47              |
| 1:AA:411:A:OP2    | 3:AD:25:ARG:NH2    | 2.47                     | 0.47              |
| 1:AA:836:G:H2'    | 1:AA:837:U:H6      | 1.79                     | 0.47              |
| 1:AA:893:C:H2'    | 1:AA:894:G:C8      | 2.49                     | 0.47              |
| 1:AA:926:G:H3'    | 1:AA:1505:G:H21    | 1.80                     | 0.47              |
| 1:AA:1260:G:OP1   | 1:AA:1284:C:H4'    | 2.14                     | 0.47              |
| 1:AA:1281:C:C5'   | 1:AA:1282:C:H5     | 2.27                     | 0.47              |
| 1:AA:1300:G:O2'   | 1:AA:1301:U:P      | 2.73                     | 0.47              |
| 2:AC:38:VAL:O     | 2:AC:42:LEU:HD23   | 2.15                     | 0.47              |
| 3:AD:25:ARG:CD    | 3:AD:26:ALA:H      | 2.24                     | 0.47              |
| 4:AE:104:ILE:HG23 | 4:AE:111:ARG:HH12  | 1.80                     | 0.47              |
| 8:AI:64:ILE:HG22  | 8:AI:65:THR:N      | 2.30                     | 0.47              |
| 10:AK:83:VAL:HG22 | 10:AK:106:ILE:HD11 | 1.97                     | 0.47              |
| 11:AL:49:ARG:HH12 | 11:AL:88:ASP:CB    | 2.27                     | 0.47              |
| 15:AP:73:ALA:HB1  | 15:AP:77:GLU:OE2   | 2.15                     | 0.47              |
| 16:AQ:10:ARG:CZ   | 16:AQ:56:ASP:H     | 2.27                     | 0.47              |
| 18:AS:51:HIS:HA   | 18:AS:55:GLN:O     | 2.15                     | 0.47              |
| 20:AB:22:TRP:CG   | 20:AB:23:ASN:N     | 2.82                     | 0.47              |
| 23:BB:189:G:P     | 46:BZ:12:ILE:HG21  | 2.55                     | 0.47              |
| 23:BB:213:A:H2'   | 23:BB:214:G:C8     | 2.50                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:309:A:H1'   | 23:BB:329:G:N3     | 2.30                     | 0.47              |
| 23:BB:528:A:N1    | 23:BB:2043:C:C5'   | 2.78                     | 0.47              |
| 23:BB:1010:A:N3   | 23:BB:1153:C:H1'   | 2.29                     | 0.47              |
| 23:BB:1081:U:H5'  | 52:BI:126:ARG:HD2  | 1.96                     | 0.47              |
| 23:BB:1367:A:H2'  | 23:BB:1368:G:H5'   | 1.95                     | 0.47              |
| 23:BB:1424:G:H2'  | 23:BB:1425:G:O4'   | 2.15                     | 0.47              |
| 23:BB:1750:G:H2'  | 23:BB:1751:U:C6    | 2.50                     | 0.47              |
| 23:BB:1775:U:H2'  | 23:BB:1776:G:O4'   | 2.14                     | 0.47              |
| 23:BB:1789:A:OP1  | 25:BC:219:VAL:HG12 | 2.14                     | 0.47              |
| 23:BB:2081:U:C5'  | 46:BZ:23:LYS:HD2   | 2.44                     | 0.47              |
| 23:BB:2800:A:N3   | 23:BB:2801:G:H1'   | 2.30                     | 0.47              |
| 25:BC:3:VAL:HG12  | 25:BC:4:LYS:N      | 2.24                     | 0.47              |
| 27:BE:156:ASN:CG  | 27:BE:157:LEU:H    | 2.23                     | 0.47              |
| 30:BH:6:LEU:HD21  | 30:BH:50:ARG:HD3   | 1.97                     | 0.47              |
| 32:BK:80:ASP:CG   | 37:BP:71:ARG:HG2   | 2.39                     | 0.47              |
| 33:BL:119:PRO:CD  | 33:BL:119:PRO:O    | 2.62                     | 0.47              |
| 39:BR:31:GLU:O    | 39:BR:32:THR:HB    | 2.15                     | 0.47              |
| 39:BR:59:ILE:O    | 39:BR:59:ILE:HG13  | 2.14                     | 0.47              |
| 1:CA:284:C:H2'    | 1:CA:285:C:H6      | 1.79                     | 0.47              |
| 1:CA:382:A:O2'    | 1:CA:383:A:H5'     | 2.15                     | 0.47              |
| 1:CA:434:U:H2'    | 1:CA:434:U:O2      | 2.14                     | 0.47              |
| 1:CA:476:U:O2'    | 1:CA:477:C:H5'     | 2.14                     | 0.47              |
| 1:CA:719:C:O2'    | 17:CR:37:LYS:HB2   | 2.15                     | 0.47              |
| 1:CA:890:G:O2'    | 1:CA:906:A:N6      | 2.48                     | 0.47              |
| 1:CA:1085:U:H3'   | 1:CA:1086:U:C6     | 2.50                     | 0.47              |
| 1:CA:1229:A:H2'   | 1:CA:1230:C:H6     | 1.79                     | 0.47              |
| 1:CA:1300:G:C2'   | 1:CA:1301:U:OP2    | 2.62                     | 0.47              |
| 1:CA:1301:U:O2'   | 1:CA:1302:C:OP1    | 2.25                     | 0.47              |
| 1:CA:1512:U:H2'   | 1:CA:1513:A:C8     | 2.50                     | 0.47              |
| 2:CC:178:ARG:HG2  | 2:CC:205:GLU:O     | 2.15                     | 0.47              |
| 3:CD:25:ARG:HH11  | 3:CD:25:ARG:CB     | 2.19                     | 0.47              |
| 4:CE:40:ASP:CG    | 4:CE:44:ARG:HB2    | 2.39                     | 0.47              |
| 4:CE:113:VAL:HG21 | 4:CE:139:THR:HG21  | 1.96                     | 0.47              |
| 7:CH:107:LYS:HB3  | 7:CH:107:LYS:NZ    | 2.30                     | 0.47              |
| 8:CI:56:MET:O     | 8:CI:58:GLU:HG2    | 2.14                     | 0.47              |
| 9:CJ:7:ARG:HD2    | 9:CJ:101:SER:OG    | 2.14                     | 0.47              |
| 11:CL:17:LYS:HB2  | 11:CL:17:LYS:HZ3   | 1.77                     | 0.47              |
| 11:CL:35:ARG:NE   | 11:CL:36:VAL:H     | 2.13                     | 0.47              |
| 11:CL:81:ILE:HD13 | 11:CL:96:THR:HG22  | 1.96                     | 0.47              |
| 17:CR:59:LYS:O    | 17:CR:63:TYR:HD2   | 1.97                     | 0.47              |
| 21:CU:41:THR:O    | 21:CU:45:LYS:HB2   | 2.15                     | 0.47              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:143:C:H2'    | 23:DB:144:A:C8     | 2.50                     | 0.47              |
| 23:DB:1060:U:OP1   | 52:DI:75:ALA:HB3   | 2.15                     | 0.47              |
| 23:DB:1332:G:H2'   | 23:DB:1332:G:N3    | 2.29                     | 0.47              |
| 23:DB:1351:C:H2'   | 23:DB:1352:U:C6    | 2.49                     | 0.47              |
| 23:DB:1541:C:H2'   | 23:DB:1542:U:C6    | 2.50                     | 0.47              |
| 23:DB:2462:C:H2'   | 23:DB:2463:C:C6    | 2.49                     | 0.47              |
| 23:DB:2597:G:OP1   | 25:DC:239:PHE:CG   | 2.68                     | 0.47              |
| 23:DB:2710:C:H2'   | 23:DB:2711:A:H8    | 1.80                     | 0.47              |
| 23:DB:2864:G:H2'   | 23:DB:2865:U:C6    | 2.49                     | 0.47              |
| 25:DC:52:HIS:O     | 25:DC:53:ILE:HD12  | 2.15                     | 0.47              |
| 25:DC:136:VAL:C    | 25:DC:138:SER:N    | 2.69                     | 0.47              |
| 26:DD:112:THR:HB   | 26:DD:167:ASN:O    | 2.14                     | 0.47              |
| 27:DE:147:LEU:HB3  | 27:DE:167:VAL:HG22 | 1.96                     | 0.47              |
| 28:DF:32:LYS:CB    | 28:DF:91:ARG:HB3   | 2.33                     | 0.47              |
| 28:DF:39:VAL:HG13  | 28:DF:84:ILE:CB    | 2.45                     | 0.47              |
| 29:DG:23:ILE:O     | 29:DG:33:THR:HA    | 2.14                     | 0.47              |
| 33:DL:59:ARG:O     | 33:DL:60:ARG:HD2   | 2.14                     | 0.47              |
| 33:DL:142:ILE:HG12 | 33:DL:144:GLU:OE1  | 2.15                     | 0.47              |
| 41:DT:21:SER:O     | 41:DT:24:MET:HB2   | 2.15                     | 0.47              |
| 41:DT:62:VAL:O     | 41:DT:63:VAL:HB    | 2.15                     | 0.47              |
| 46:DZ:1:MET:HA     | 46:DZ:9:TYR:CG     | 2.50                     | 0.47              |
| 46:DZ:39:LYS:HD3   | 46:DZ:61:ASN:CG    | 2.39                     | 0.47              |
| 46:DZ:59:ARG:O     | 46:DZ:61:ASN:N     | 2.41                     | 0.47              |
| 47:D0:29:VAL:HG22  | 47:D0:30:ASP:N     | 2.28                     | 0.47              |
| 47:D0:36:LYS:HG2   | 47:D0:37:HIS:O     | 2.15                     | 0.47              |
| 49:D2:18:PHE:CE2   | 49:D2:44:VAL:HB    | 2.50                     | 0.47              |
| 50:D3:25:HIS:O     | 50:D3:27:ASN:N     | 2.48                     | 0.47              |
| 52:DI:45:THR:O     | 52:DI:48:ILE:HG22  | 2.14                     | 0.47              |
| 52:DI:69:VAL:O     | 52:DI:69:VAL:HG23  | 2.15                     | 0.47              |
| 1:AA:263:A:P       | 19:AT:73:ARG:HH22  | 2.38                     | 0.47              |
| 1:AA:513:C:H2'     | 1:AA:514:C:H6      | 1.79                     | 0.47              |
| 1:AA:768:A:H4'     | 1:AA:1523:G:N2     | 2.30                     | 0.47              |
| 1:AA:803:G:H2'     | 1:AA:804:U:C6      | 2.50                     | 0.47              |
| 1:AA:1112:C:O2     | 2:AC:178:ARG:N     | 2.48                     | 0.47              |
| 1:AA:1117:A:H4'    | 8:AI:105:ARG:NH1   | 2.30                     | 0.47              |
| 1:AA:1226:C:P      | 12:AM:89:ARG:HH12  | 2.37                     | 0.47              |
| 2:AC:76:ILE:O      | 2:AC:83:VAL:HG23   | 2.14                     | 0.47              |
| 2:AC:90:VAL:HA     | 2:AC:93:ILE:CG2    | 2.44                     | 0.47              |
| 3:AD:54:LEU:O      | 3:AD:57:LYS:HB3    | 2.14                     | 0.47              |
| 3:AD:71:PHE:HA     | 3:AD:74:TYR:HD2    | 1.80                     | 0.47              |
| 19:AT:57:VAL:HG12  | 19:AT:57:VAL:O     | 2.15                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:AB:15:PHE:HD1   | 20:AB:16:GLY:H     | 1.63                     | 0.47              |
| 23:BB:55:G:H2'     | 23:BB:56:A:C8      | 2.50                     | 0.47              |
| 23:BB:236:C:O2'    | 23:BB:237:C:H5'    | 2.14                     | 0.47              |
| 23:BB:527:C:C4     | 23:BB:2779:U:H2'   | 2.50                     | 0.47              |
| 23:BB:599:A:O2'    | 23:BB:600:G:H5'    | 2.15                     | 0.47              |
| 23:BB:664:G:O2'    | 23:BB:665:U:H5'    | 2.15                     | 0.47              |
| 23:BB:1710:G:O2'   | 23:BB:1711:A:H5'   | 2.14                     | 0.47              |
| 23:BB:2023:C:H4'   | 23:BB:2617:U:O3'   | 2.15                     | 0.47              |
| 23:BB:2038:G:H2'   | 23:BB:2039:U:C6    | 2.49                     | 0.47              |
| 23:BB:2519:U:H5'   | 23:BB:2567:G:N2    | 2.30                     | 0.47              |
| 23:BB:2603:G:O2'   | 23:BB:2604:U:H5'   | 2.15                     | 0.47              |
| 23:BB:2773:C:O2'   | 23:BB:2774:C:H5'   | 2.15                     | 0.47              |
| 25:BC:224:MET:HB3  | 25:BC:233:GLY:H    | 1.80                     | 0.47              |
| 29:BG:32:LEU:HD21  | 29:BG:74:MET:HB3   | 1.97                     | 0.47              |
| 30:BH:121:VAL:HG11 | 30:BH:128:HIS:CD2  | 2.49                     | 0.47              |
| 31:BJ:7:LYS:NZ     | 31:BJ:49:ASP:H     | 2.12                     | 0.47              |
| 32:BK:40:LYS:HZ2   | 32:BK:89:ASN:HD21  | 1.63                     | 0.47              |
| 32:BK:73:ASP:OD1   | 32:BK:74:GLY:N     | 2.48                     | 0.47              |
| 33:BL:34:GLY:O     | 33:BL:35:HIS:C     | 2.57                     | 0.47              |
| 33:BL:39:LYS:HB2   | 33:BL:46:VAL:HG13  | 1.96                     | 0.47              |
| 34:BM:103:TYR:O    | 34:BM:105:MET:N    | 2.48                     | 0.47              |
| 34:BM:116:ALA:O    | 34:BM:119:LEU:HD23 | 2.15                     | 0.47              |
| 36:BO:26:LEU:HG    | 36:BO:39:VAL:HG22  | 1.96                     | 0.47              |
| 39:BR:78:ARG:HD3   | 39:BR:87:GLN:C     | 2.40                     | 0.47              |
| 44:BX:22:LEU:CD2   | 44:BX:25:GLN:HB3   | 2.45                     | 0.47              |
| 47:B0:36:LYS:HA    | 47:B0:41:HIS:C     | 2.40                     | 0.47              |
| 52:BI:83:ALA:N     | 52:BI:100:ILE:HD11 | 2.29                     | 0.47              |
| 1:CA:197:A:H4'     | 1:CA:198:G:O5'     | 2.15                     | 0.47              |
| 1:CA:252:U:H2'     | 1:CA:253:A:C8      | 2.49                     | 0.47              |
| 1:CA:647:C:O2'     | 1:CA:648:A:H5'     | 2.15                     | 0.47              |
| 1:CA:695:A:H5'     | 10:CK:52:ARG:NH2   | 2.28                     | 0.47              |
| 1:CA:1225:A:H5'    | 12:CM:101:THR:HG1  | 1.80                     | 0.47              |
| 12:CM:95:PRO:CD    | 12:CM:108:ARG:HG2  | 2.45                     | 0.47              |
| 14:CO:23:SER:HB3   | 14:CO:26:VAL:CG2   | 2.45                     | 0.47              |
| 15:CP:53:ASP:O     | 15:CP:57:ILE:HG22  | 2.14                     | 0.47              |
| 17:CR:20:ILE:O     | 17:CR:20:ILE:HG12  | 2.15                     | 0.47              |
| 18:CS:14:LEU:HD12  | 18:CS:15:LEU:N     | 2.30                     | 0.47              |
| 20:CB:199:ILE:HG13 | 20:CB:199:ILE:O    | 2.15                     | 0.47              |
| 23:DB:5:A:H2'      | 23:DB:6:A:C8       | 2.50                     | 0.47              |
| 23:DB:129:C:H4'    | 23:DB:1348:C:O2'   | 2.15                     | 0.47              |
| 23:DB:543:G:C2'    | 23:DB:545:U:OP1    | 2.63                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DB:599:A:O2'    | 23:DB:600:G:H5'   | 2.15                     | 0.47              |
| 23:DB:962:G:O2'    | 23:DB:963:U:H5'   | 2.15                     | 0.47              |
| 23:DB:1009:A:H5'   | 38:DQ:58:GLN:HE21 | 1.80                     | 0.47              |
| 23:DB:1355:G:O2'   | 23:DB:1356:G:H5'  | 2.14                     | 0.47              |
| 23:DB:1427:A:H4'   | 23:DB:1428:C:O4'  | 2.14                     | 0.47              |
| 23:DB:1665:A:H5''  | 32:DK:66:LYS:HB3  | 1.97                     | 0.47              |
| 23:DB:1710:G:O2'   | 23:DB:1711:A:H5'  | 2.14                     | 0.47              |
| 23:DB:1720:U:O2'   | 23:DB:1721:G:H5'  | 2.15                     | 0.47              |
| 23:DB:1882:U:O2'   | 23:DB:1883:U:H5'  | 2.14                     | 0.47              |
| 23:DB:2093:G:O2'   | 23:DB:2094:A:H5'  | 2.14                     | 0.47              |
| 23:DB:2722:G:H2'   | 23:DB:2723:C:C6   | 2.49                     | 0.47              |
| 23:DB:2733:A:H3'   | 23:DB:2733:A:C8   | 2.50                     | 0.47              |
| 23:DB:2801:G:H2'   | 23:DB:2802:G:C8   | 2.50                     | 0.47              |
| 25:DC:52:HIS:O     | 25:DC:53:ILE:CB   | 2.61                     | 0.47              |
| 26:DD:50:VAL:HG13  | 26:DD:77:ARG:O    | 2.14                     | 0.47              |
| 27:DE:123:LYS:NZ   | 27:DE:158:PHE:HA  | 2.30                     | 0.47              |
| 27:DE:169:VAL:HG22 | 27:DE:171:ASP:H   | 1.80                     | 0.47              |
| 28:DF:56:LEU:HD13  | 28:DF:88:VAL:HG21 | 1.97                     | 0.47              |
| 28:DF:177:ARG:O    | 28:DF:178:LYS:HB2 | 2.15                     | 0.47              |
| 29:DG:8:VAL:HG12   | 29:DG:49:LEU:HD12 | 1.96                     | 0.47              |
| 29:DG:10:VAL:HG11  | 29:DG:44:HIS:CE1  | 2.50                     | 0.47              |
| 29:DG:25:ILE:CD1   | 29:DG:75:VAL:HG22 | 2.45                     | 0.47              |
| 30:DH:88:GLY:O     | 30:DH:124:THR:HA  | 2.15                     | 0.47              |
| 31:DJ:67:ASN:C     | 31:DJ:69:ARG:N    | 2.73                     | 0.47              |
| 31:DJ:93:ILE:HG22  | 31:DJ:93:ILE:O    | 2.15                     | 0.47              |
| 34:DM:62:LYS:H     | 34:DM:104:GLU:CB  | 2.22                     | 0.47              |
| 36:DO:35:ILE:CG2   | 36:DO:74:VAL:HG21 | 2.44                     | 0.47              |
| 37:DP:65:ASN:H     | 37:DP:71:ARG:CA   | 2.27                     | 0.47              |
| 38:DQ:82:LEU:HG    | 38:DQ:88:GLU:CG   | 2.45                     | 0.47              |
| 38:DQ:116:LEU:HD22 | 38:DQ:116:LEU:H   | 1.79                     | 0.47              |
| 41:DT:40:LYS:HE3   | 41:DT:59:ASN:O    | 2.14                     | 0.47              |
| 1:AA:108:G:C6      | 19:AT:9:ARG:HG2   | 2.50                     | 0.47              |
| 1:AA:284:C:H2'     | 1:AA:285:C:H6     | 1.79                     | 0.47              |
| 1:AA:413:G:H5'     | 1:AA:414:A:OP1    | 2.14                     | 0.47              |
| 1:AA:589:U:O2'     | 1:AA:590:U:H5'    | 2.14                     | 0.47              |
| 1:AA:652:U:H1'     | 1:AA:653:U:C5     | 2.50                     | 0.47              |
| 1:AA:1111:A:C2     | 2:AC:176:THR:HG23 | 2.50                     | 0.47              |
| 1:AA:1129:C:O2'    | 1:AA:1139:G:N7    | 2.42                     | 0.47              |
| 1:AA:1212:U:H5'    | 1:AA:1213:A:O4'   | 2.15                     | 0.47              |
| 1:AA:1406:U:H3'    | 1:AA:1407:C:H6    | 1.79                     | 0.47              |
| 2:AC:53:ARG:HG2    | 2:AC:54:ILE:N     | 2.26                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:AC:115:VAL:CG1  | 2:AC:137:VAL:HG13  | 2.44                     | 0.47              |
| 4:AE:105:ILE:HB   | 4:AE:123:LEU:CA    | 2.44                     | 0.47              |
| 5:AF:51:ILE:O     | 5:AF:51:ILE:HG23   | 2.15                     | 0.47              |
| 8:AI:66:VAL:HG21  | 8:AI:74:GLN:HG3    | 1.97                     | 0.47              |
| 11:AL:35:ARG:HE   | 11:AL:35:ARG:CA    | 2.23                     | 0.47              |
| 11:AL:58:ASN:ND2  | 11:AL:58:ASN:H     | 2.12                     | 0.47              |
| 14:AO:70:LYS:HZ3  | 14:AO:74:VAL:CG1   | 2.28                     | 0.47              |
| 15:AP:67:ILE:CD1  | 15:AP:72:ALA:HA    | 2.45                     | 0.47              |
| 16:AQ:56:ASP:CG   | 16:AQ:80:LYS:HA    | 2.39                     | 0.47              |
| 16:AQ:79:GLU:HG3  | 16:AQ:80:LYS:N     | 2.31                     | 0.47              |
| 18:AS:69:LYS:O    | 18:AS:72:GLU:HB2   | 2.15                     | 0.47              |
| 19:AT:34:VAL:HG11 | 19:AT:78:LEU:HD13  | 1.97                     | 0.47              |
| 20:AB:9:LEU:HD22  | 20:AB:10:LYS:N     | 2.30                     | 0.47              |
| 22:BA:105:G:O2'   | 22:BA:106:G:H5'    | 2.15                     | 0.47              |
| 23:BB:173:A:H2'   | 23:BB:174:U:H6     | 1.80                     | 0.47              |
| 23:BB:327:G:H2'   | 23:BB:328:U:C6     | 2.50                     | 0.47              |
| 23:BB:535:G:H3'   | 55:BB:3420:HOH:O   | 2.15                     | 0.47              |
| 23:BB:657:U:H2'   | 23:BB:658:U:C6     | 2.50                     | 0.47              |
| 23:BB:661:A:O2'   | 33:BL:23:ILE:HG23  | 2.14                     | 0.47              |
| 23:BB:764:A:OP2   | 25:BC:213:ARG:NH2  | 2.47                     | 0.47              |
| 23:BB:1515:A:H5'  | 23:BB:1557:C:C5'   | 2.44                     | 0.47              |
| 23:BB:2299:U:H2'  | 23:BB:2300:C:C6    | 2.50                     | 0.47              |
| 23:BB:2543:G:H2'  | 23:BB:2544:G:C8    | 2.50                     | 0.47              |
| 25:BC:244:VAL:O   | 25:BC:245:THR:C    | 2.58                     | 0.47              |
| 26:BD:29:VAL:HG12 | 26:BD:185:ASN:ND2  | 2.30                     | 0.47              |
| 26:BD:45:TYR:CE2  | 26:BD:83:ARG:HG3   | 2.50                     | 0.47              |
| 26:BD:122:VAL:CB  | 26:BD:141:ARG:HH12 | 2.28                     | 0.47              |
| 30:BH:30:LEU:HD13 | 30:BH:35:LYS:HD3   | 1.97                     | 0.47              |
| 30:BH:114:GLU:HB3 | 30:BH:133:GLN:C    | 2.40                     | 0.47              |
| 31:BJ:63:ALA:HA   | 31:BJ:69:ARG:HD3   | 1.97                     | 0.47              |
| 34:BM:21:ALA:O    | 34:BM:96:ILE:HG13  | 2.15                     | 0.47              |
| 35:BN:49:GLU:O    | 35:BN:52:ILE:HB    | 2.15                     | 0.47              |
| 35:BN:99:LYS:HB3  | 35:BN:99:LYS:HZ2   | 1.75                     | 0.47              |
| 35:BN:103:ARG:HB2 | 35:BN:110:MET:SD   | 2.55                     | 0.47              |
| 36:BO:84:GLU:OE1  | 36:BO:85:LYS:HG3   | 2.14                     | 0.47              |
| 38:BQ:20:ALA:O    | 38:BQ:22:GLY:N     | 2.48                     | 0.47              |
| 38:BQ:35:PHE:HE1  | 39:BR:85:LYS:HZ2   | 1.63                     | 0.47              |
| 39:BR:5:PHE:HB3   | 39:BR:12:HIS:CG    | 2.50                     | 0.47              |
| 41:BT:48:GLN:HG3  | 41:BT:49:LYS:N     | 2.30                     | 0.47              |
| 44:BX:36:GLN:O    | 44:BX:37:LEU:HD23  | 2.15                     | 0.47              |
| 44:BX:38:GLN:HG2  | 44:BX:39:GLN:N     | 2.29                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:BZ:49:ARG:O    | 46:BZ:51:VAL:HG23 | 2.14                     | 0.47              |
| 47:B0:42:ILE:HD11 | 47:B0:44:ALA:HB3  | 1.97                     | 0.47              |
| 48:B1:31:GLU:O    | 48:B1:33:LEU:HG   | 2.15                     | 0.47              |
| 50:B3:56:LEU:O    | 50:B3:57:VAL:HB   | 2.15                     | 0.47              |
| 52:BI:29:GLN:HE21 | 52:BI:29:GLN:HA   | 1.80                     | 0.47              |
| 1:CA:840:C:N3     | 1:CA:842:U:H4'    | 2.30                     | 0.47              |
| 1:CA:948:C:OP1    | 12:CM:105:ALA:HA  | 2.14                     | 0.47              |
| 1:CA:992:U:H1'    | 1:CA:993:G:C2     | 2.49                     | 0.47              |
| 3:CD:13:ARG:O     | 3:CD:13:ARG:HG3   | 2.15                     | 0.47              |
| 4:CE:45:VAL:O     | 4:CE:71:ILE:HG22  | 2.14                     | 0.47              |
| 6:CG:29:LEU:HD12  | 6:CG:42:VAL:HG22  | 1.96                     | 0.47              |
| 6:CG:100:MET:O    | 6:CG:104:VAL:HG23 | 2.14                     | 0.47              |
| 12:CM:21:ILE:O    | 12:CM:22:TYR:C    | 2.57                     | 0.47              |
| 23:DB:299:A:H2    | 23:DB:319:G:N3    | 2.13                     | 0.47              |
| 23:DB:346:A:N7    | 23:DB:347:A:H1'   | 2.30                     | 0.47              |
| 23:DB:657:U:H2'   | 23:DB:658:U:C6    | 2.50                     | 0.47              |
| 23:DB:802:A:H4'   | 55:DB:3289:HOH:O  | 2.15                     | 0.47              |
| 23:DB:902:C:O2'   | 23:DB:903:C:H5'   | 2.15                     | 0.47              |
| 23:DB:962:G:O2'   | 23:DB:2250:G:N2   | 2.48                     | 0.47              |
| 23:DB:1098:A:O5'  | 52:DI:3:LYS:CG    | 2.63                     | 0.47              |
| 23:DB:1199:U:C2   | 23:DB:1200:C:C5   | 3.03                     | 0.47              |
| 23:DB:1409:U:O2'  | 23:DB:1410:G:H5'  | 2.15                     | 0.47              |
| 23:DB:2071:A:H2'  | 23:DB:2072:C:H6   | 1.76                     | 0.47              |
| 23:DB:2300:C:H2'  | 23:DB:2301:C:H6   | 1.79                     | 0.47              |
| 25:DC:12:ARG:HH11 | 25:DC:18:VAL:CB   | 2.28                     | 0.47              |
| 27:DE:88:ARG:HB3  | 27:DE:89:PRO:HD2  | 1.97                     | 0.47              |
| 30:DH:67:ALA:C    | 30:DH:69:ALA:H    | 2.23                     | 0.47              |
| 30:DH:68:ARG:HD3  | 30:DH:71:LYS:HD3  | 1.97                     | 0.47              |
| 34:DM:33:LEU:CD2  | 34:DM:124:LEU:HB2 | 2.44                     | 0.47              |
| 35:DN:96:ARG:HH11 | 35:DN:96:ARG:HG2  | 1.79                     | 0.47              |
| 40:DS:7:HIS:NE2   | 40:DS:10:ALA:HA   | 2.29                     | 0.47              |
| 42:DU:72:PHE:CD2  | 42:DU:74:ALA:HB3  | 2.50                     | 0.47              |
| 1:AA:216:U:H2'    | 1:AA:217:C:C6     | 2.50                     | 0.46              |
| 1:AA:455:G:H2'    | 1:AA:456:A:C8     | 2.51                     | 0.46              |
| 1:AA:601:G:H2'    | 1:AA:602:A:H8     | 1.80                     | 0.46              |
| 1:AA:691:G:H1'    | 1:AA:696:A:N6     | 2.30                     | 0.46              |
| 1:AA:909:A:H2'    | 1:AA:910:C:O4'    | 2.14                     | 0.46              |
| 1:AA:1432:G:C5'   | 37:BP:106:ALA:HB2 | 2.44                     | 0.46              |
| 1:AA:1456:A:H2'   | 1:AA:1457:G:O4'   | 2.16                     | 0.46              |
| 3:AD:24:VAL:HG23  | 3:AD:25:ARG:HD2   | 1.96                     | 0.46              |
| 3:AD:119:HIS:C    | 3:AD:121:ALA:H    | 2.22                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:AD:196:GLU:HA    | 3:AD:199:ILE:HD12  | 1.97                     | 0.46              |
| 7:AH:64:TYR:CA     | 7:AH:70:VAL:HG23   | 2.44                     | 0.46              |
| 7:AH:69:ALA:HB3    | 7:AH:72:GLU:OE2    | 2.15                     | 0.46              |
| 8:AI:18:VAL:HG13   | 8:AI:64:ILE:HG12   | 1.96                     | 0.46              |
| 9:AJ:73:LEU:O      | 9:AJ:74:VAL:HB     | 2.15                     | 0.46              |
| 11:AL:1:ALA:HB1    | 11:AL:5:GLN:HB2    | 1.98                     | 0.46              |
| 11:AL:89:LEU:N     | 11:AL:89:LEU:HD22  | 2.30                     | 0.46              |
| 12:AM:70:ARG:NE    | 28:BF:112:ASP:OD2  | 2.49                     | 0.46              |
| 13:AN:14:ALA:O     | 13:AN:18:LYS:HG2   | 2.15                     | 0.46              |
| 13:AN:72:PHE:CE2   | 13:AN:77:GLY:HA2   | 2.50                     | 0.46              |
| 14:AO:17:ASP:HB2   | 14:AO:18:ALA:H     | 1.57                     | 0.46              |
| 16:AQ:10:ARG:NE    | 16:AQ:10:ARG:CA    | 2.77                     | 0.46              |
| 23:BB:6:A:O2'      | 23:BB:7:G:H5'      | 2.15                     | 0.46              |
| 23:BB:135:U:H2'    | 23:BB:136:G:N9     | 2.29                     | 0.46              |
| 23:BB:241:A:H8     | 23:BB:241:A:OP1    | 1.98                     | 0.46              |
| 23:BB:528:A:C6     | 23:BB:2042:A:H2'   | 2.46                     | 0.46              |
| 23:BB:778:G:H5''   | 25:BC:48:ILE:HD12  | 1.97                     | 0.46              |
| 23:BB:946:C:H2'    | 23:BB:947:A:H8     | 1.80                     | 0.46              |
| 23:BB:1029:A:H2'   | 23:BB:1030:C:O4'   | 2.15                     | 0.46              |
| 23:BB:1156:A:N6    | 38:BQ:47:ARG:HD2   | 2.30                     | 0.46              |
| 23:BB:1257:C:H5'   | 27:BE:78:TRP:CH2   | 2.49                     | 0.46              |
| 23:BB:1409:U:O2'   | 23:BB:1410:G:H5'   | 2.15                     | 0.46              |
| 23:BB:2378:A:C2'   | 23:BB:2379:G:H5'   | 2.43                     | 0.46              |
| 23:BB:2769:U:O2'   | 23:BB:2770:G:H5'   | 2.16                     | 0.46              |
| 24:BV:82:TYR:CB    | 34:BM:36:VAL:HG12  | 2.45                     | 0.46              |
| 25:BC:160:TYR:HA   | 25:BC:193:GLU:HG2  | 1.96                     | 0.46              |
| 26:BD:145:SER:C    | 26:BD:146:ILE:HD12 | 2.40                     | 0.46              |
| 27:BE:149:ILE:HD11 | 27:BE:186:VAL:HG13 | 1.97                     | 0.46              |
| 27:BE:173:THR:O    | 27:BE:175:ILE:HG22 | 2.14                     | 0.46              |
| 31:BJ:132:HIS:C    | 31:BJ:134:ALA:H    | 2.22                     | 0.46              |
| 34:BM:43:ALA:C     | 34:BM:45:GLN:H     | 2.23                     | 0.46              |
| 34:BM:108:VAL:O    | 34:BM:112:LEU:HD13 | 2.15                     | 0.46              |
| 34:BM:108:VAL:C    | 34:BM:112:LEU:HD13 | 2.40                     | 0.46              |
| 35:BN:27:SER:OG    | 35:BN:34:ILE:HG21  | 2.15                     | 0.46              |
| 35:BN:72:ASP:C     | 35:BN:74:GLU:H     | 2.24                     | 0.46              |
| 35:BN:99:LYS:HB3   | 35:BN:99:LYS:HZ3   | 1.79                     | 0.46              |
| 36:BO:66:GLY:O     | 36:BO:67:ASN:ND2   | 2.48                     | 0.46              |
| 40:BS:24:ILE:HD13  | 40:BS:36:LEU:HD11  | 1.97                     | 0.46              |
| 42:BU:62:ALA:O     | 42:BU:63:ALA:C     | 2.58                     | 0.46              |
| 43:BW:58:LEU:HA    | 43:BW:79:ILE:CG2   | 2.45                     | 0.46              |
| 46:BZ:8:LYS:CD     | 46:BZ:9:TYR:N      | 2.70                     | 0.46              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:B3:34:LYS:HB3   | 50:B3:35:LYS:NZ    | 2.30                     | 0.46              |
| 1:CA:216:U:H2'     | 1:CA:217:C:C6      | 2.50                     | 0.46              |
| 1:CA:279:A:H5'     | 1:CA:281:G:O4'     | 2.15                     | 0.46              |
| 1:CA:472:U:N3      | 1:CA:473:U:C4      | 2.82                     | 0.46              |
| 1:CA:601:G:H2'     | 1:CA:602:A:C8      | 2.50                     | 0.46              |
| 1:CA:831:A:O2'     | 1:CA:832:G:H5'     | 2.15                     | 0.46              |
| 1:CA:1028:C:H2'    | 1:CA:1029:U:C6     | 2.49                     | 0.46              |
| 1:CA:1363:A:H2'    | 1:CA:1363:A:N3     | 2.30                     | 0.46              |
| 2:CC:13:ILE:HG13   | 2:CC:177:LEU:HB3   | 1.98                     | 0.46              |
| 2:CC:176:THR:HG1   | 2:CC:179:ALA:HB2   | 1.79                     | 0.46              |
| 7:CH:46:GLU:N      | 7:CH:63:LYS:HE3    | 2.30                     | 0.46              |
| 8:CI:115:VAL:HG21  | 9:CJ:62:ARG:HG3    | 1.97                     | 0.46              |
| 9:CJ:65:TYR:HB3    | 13:CN:95:LEU:HD11  | 1.96                     | 0.46              |
| 10:CK:127:ARG:HH11 | 10:CK:127:ARG:HG3  | 1.79                     | 0.46              |
| 12:CM:105:ALA:O    | 12:CM:109:LYS:HG3  | 2.15                     | 0.46              |
| 13:CN:10:VAL:HG12  | 13:CN:11:LYS:NZ    | 2.30                     | 0.46              |
| 16:CQ:82:VAL:C     | 16:CQ:83:LEU:HD22  | 2.40                     | 0.46              |
| 20:CB:18:GLN:HB2   | 20:CB:188:THR:OG1  | 2.14                     | 0.46              |
| 23:DB:64:A:H5'     | 41:DT:76:ARG:HD2   | 1.95                     | 0.46              |
| 23:DB:356:G:H2'    | 23:DB:357:C:H6     | 1.80                     | 0.46              |
| 23:DB:358:U:H2'    | 23:DB:359:G:H8     | 1.77                     | 0.46              |
| 23:DB:533:G:N3     | 38:DQ:40:LYS:HG2   | 2.30                     | 0.46              |
| 23:DB:631:A:O2'    | 33:DL:66:PHE:HD1   | 1.97                     | 0.46              |
| 23:DB:957:C:O2'    | 23:DB:958:U:H5''   | 2.14                     | 0.46              |
| 23:DB:1048:A:C5    | 23:DB:1111:A:C2    | 3.03                     | 0.46              |
| 23:DB:1098:A:HO2'  | 52:DI:4:VAL:C      | 2.22                     | 0.46              |
| 23:DB:1669:A:H2'   | 23:DB:1669:A:N3    | 2.31                     | 0.46              |
| 23:DB:1936:A:H2    | 23:DB:1943:U:C5    | 2.33                     | 0.46              |
| 23:DB:1997:C:H5'   | 26:DD:128:ARG:NH2  | 2.29                     | 0.46              |
| 23:DB:1999:C:O2'   | 23:DB:2000:C:H5'   | 2.15                     | 0.46              |
| 23:DB:2300:C:H2'   | 23:DB:2301:C:C6    | 2.51                     | 0.46              |
| 23:DB:2420:C:H3'   | 50:D3:31:ILE:HG22  | 1.96                     | 0.46              |
| 24:DV:69:GLU:O     | 24:DV:70:ILE:HG23  | 2.15                     | 0.46              |
| 25:DC:38:LYS:O     | 25:DC:60:ALA:HA    | 2.14                     | 0.46              |
| 25:DC:77:VAL:HG23  | 25:DC:113:ASP:HB2  | 1.97                     | 0.46              |
| 27:DE:153:LEU:HD23 | 27:DE:172:ALA:N    | 2.31                     | 0.46              |
| 28:DF:79:ARG:HB2   | 28:DF:82:TYR:CZ    | 2.50                     | 0.46              |
| 31:DJ:43:GLU:CA    | 38:DQ:63:ARG:HH12  | 2.28                     | 0.46              |
| 31:DJ:100:VAL:HG13 | 31:DJ:101:ILE:HG12 | 1.96                     | 0.46              |
| 33:DL:108:ALA:HB3  | 33:DL:125:LEU:HB3  | 1.97                     | 0.46              |
| 33:DL:123:ARG:HA   | 33:DL:142:ILE:CA   | 2.45                     | 0.46              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:DM:4:PRO:HB2   | 34:DM:69:PRO:CG    | 2.45                     | 0.46              |
| 34:DM:96:ILE:HG22 | 34:DM:97:GLN:CD    | 2.39                     | 0.46              |
| 35:DN:12:ARG:HD3  | 35:DN:12:ARG:N     | 2.29                     | 0.46              |
| 40:DS:4:ILE:HG12  | 40:DS:106:VAL:HG12 | 1.97                     | 0.46              |
| 40:DS:7:HIS:NE2   | 40:DS:46:LEU:HD22  | 2.30                     | 0.46              |
| 42:DU:90:LYS:O    | 42:DU:91:LYS:HB2   | 2.16                     | 0.46              |
| 42:DU:96:LYS:O    | 42:DU:97:SER:HB3   | 2.13                     | 0.46              |
| 47:D0:32:THR:HG21 | 47:D0:41:HIS:CE1   | 2.49                     | 0.46              |
| 47:D0:42:ILE:O    | 47:D0:43:THR:C     | 2.57                     | 0.46              |
| 47:D0:50:GLY:O    | 47:D0:51:ARG:C     | 2.57                     | 0.46              |
| 48:D1:7:LYS:HA    | 48:D1:26:LYS:HA    | 1.97                     | 0.46              |
| 48:D1:15:GLY:HA3  | 48:D1:47:ILE:CG2   | 2.44                     | 0.46              |
| 52:DI:37:PHE:CE1  | 52:DI:58:ILE:HD11  | 2.50                     | 0.46              |
| 1:AA:239:U:H5''   | 1:AA:239:U:H6      | 1.80                     | 0.46              |
| 1:AA:393:A:H5'    | 1:AA:483:C:O2'     | 2.15                     | 0.46              |
| 1:AA:478:A:H2'    | 1:AA:479:U:O4'     | 2.15                     | 0.46              |
| 1:AA:676:A:H1'    | 10:AK:116:PRO:HB3  | 1.96                     | 0.46              |
| 1:AA:691:G:H2'    | 1:AA:692:U:C6      | 2.50                     | 0.46              |
| 1:AA:754:C:H3'    | 1:AA:754:C:O2      | 2.15                     | 0.46              |
| 1:AA:889:A:H61    | 1:AA:907:A:H3'     | 1.80                     | 0.46              |
| 1:AA:1390:U:H2'   | 1:AA:1391:U:H6     | 1.79                     | 0.46              |
| 9:AJ:88:MET:HB2   | 9:AJ:89:ARG:HH22   | 1.81                     | 0.46              |
| 10:AK:126:ARG:CB  | 21:AU:33:ARG:HD2   | 2.39                     | 0.46              |
| 20:AB:115:ASP:O   | 20:AB:119:GLN:HG2  | 2.15                     | 0.46              |
| 23:BB:443:A:H5''  | 27:BE:44:ARG:HH12  | 1.80                     | 0.46              |
| 23:BB:834:G:H2'   | 23:BB:835:C:H6     | 1.79                     | 0.46              |
| 23:BB:1190:G:OP1  | 33:BL:41:ARG:NE    | 2.48                     | 0.46              |
| 23:BB:1526:C:H2'  | 23:BB:1527:G:O4'   | 2.15                     | 0.46              |
| 23:BB:2263:C:H2'  | 23:BB:2264:C:C6    | 2.50                     | 0.46              |
| 23:BB:2477:U:H4'  | 23:BB:2479:U:O4    | 2.16                     | 0.46              |
| 23:BB:2733:A:C8   | 23:BB:2733:A:H3'   | 2.50                     | 0.46              |
| 25:BC:16:VAL:C    | 25:BC:17:LYS:HD2   | 2.40                     | 0.46              |
| 25:BC:32:LEU:HD13 | 25:BC:61:TYR:CE1   | 2.50                     | 0.46              |
| 25:BC:53:ILE:HG21 | 25:BC:218:THR:HG23 | 1.95                     | 0.46              |
| 25:BC:59:GLN:HB3  | 25:BC:60:ALA:H     | 1.51                     | 0.46              |
| 25:BC:159:THR:C   | 25:BC:160:TYR:HD2  | 2.23                     | 0.46              |
| 26:BD:139:SER:O   | 26:BD:140:HIS:C    | 2.58                     | 0.46              |
| 28:BF:115:GLY:HA3 | 28:BF:177:ARG:N    | 2.31                     | 0.46              |
| 29:BG:28:LYS:C    | 29:BG:29:ASN:HD22  | 2.23                     | 0.46              |
| 31:BJ:102:GLU:OE2 | 31:BJ:124:VAL:HG11 | 2.16                     | 0.46              |
| 32:BK:98:ARG:HA   | 32:BK:118:LEU:CD2  | 2.45                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:BK:114:LYS:O   | 32:BK:117:SER:HB3  | 2.15                     | 0.46              |
| 35:BN:19:ALA:C    | 35:BN:21:PHE:N     | 2.72                     | 0.46              |
| 35:BN:45:ARG:N    | 35:BN:45:ARG:HD2   | 2.30                     | 0.46              |
| 36:BO:6:ALA:C     | 36:BO:8:ILE:H      | 2.23                     | 0.46              |
| 36:BO:6:ALA:HB1   | 36:BO:10:ARG:NH1   | 2.30                     | 0.46              |
| 36:BO:57:ALA:HB3  | 36:BO:62:LEU:HA    | 1.97                     | 0.46              |
| 38:BQ:85:ALA:HB3  | 38:BQ:88:GLU:O     | 2.15                     | 0.46              |
| 38:BQ:105:PHE:O   | 38:BQ:109:VAL:HG13 | 2.15                     | 0.46              |
| 40:BS:89:ALA:O    | 40:BS:90:LYS:HD2   | 2.16                     | 0.46              |
| 41:BT:44:LYS:HB2  | 41:BT:44:LYS:NZ    | 2.30                     | 0.46              |
| 43:BW:23:LYS:HG3  | 43:BW:24:ARG:N     | 2.30                     | 0.46              |
| 49:B2:14:ARG:O    | 49:B2:14:ARG:HD3   | 2.14                     | 0.46              |
| 52:BI:21:PRO:CB   | 52:BI:22:PRO:HD3   | 2.42                     | 0.46              |
| 52:BI:44:LYS:O    | 52:BI:48:ILE:HG13  | 2.15                     | 0.46              |
| 1:CA:547:A:H4'    | 1:CA:548:G:O5'     | 2.16                     | 0.46              |
| 1:CA:782:A:H2'    | 1:CA:783:C:O4'     | 2.14                     | 0.46              |
| 1:CA:1049:U:H1'   | 1:CA:1201:A:N7     | 2.30                     | 0.46              |
| 1:CA:1118:U:H2'   | 1:CA:1119:C:C6     | 2.47                     | 0.46              |
| 1:CA:1368:A:O2'   | 1:CA:1369:C:H5'    | 2.15                     | 0.46              |
| 2:CC:190:THR:HG22 | 2:CC:191:THR:N     | 2.31                     | 0.46              |
| 3:CD:59:LYS:O     | 3:CD:63:ILE:HG22   | 2.15                     | 0.46              |
| 10:CK:74:LYS:C    | 10:CK:76:TYR:H     | 2.23                     | 0.46              |
| 16:CQ:44:HIS:HB2  | 16:CQ:69:THR:O     | 2.15                     | 0.46              |
| 19:CT:67:HIS:CG   | 19:CT:68:LYS:H     | 2.31                     | 0.46              |
| 22:DA:13:G:C2'    | 22:DA:14:U:H5''    | 2.45                     | 0.46              |
| 23:DB:106:C:H2'   | 23:DB:107:G:C8     | 2.51                     | 0.46              |
| 23:DB:146:A:H2'   | 23:DB:147:C:H6     | 1.80                     | 0.46              |
| 23:DB:286:U:H2'   | 23:DB:287:G:C8     | 2.51                     | 0.46              |
| 23:DB:448:U:O4'   | 23:DB:448:U:OP2    | 2.34                     | 0.46              |
| 23:DB:753:A:H2'   | 23:DB:754:U:H6     | 1.78                     | 0.46              |
| 23:DB:931:U:N3    | 23:DB:1166:G:N2    | 2.63                     | 0.46              |
| 23:DB:1720:U:C2'  | 23:DB:1721:G:H5'   | 2.46                     | 0.46              |
| 23:DB:1735:A:H2'  | 23:DB:1736:U:C6    | 2.50                     | 0.46              |
| 23:DB:1820:U:O2'  | 25:DC:157:ALA:HB3  | 2.15                     | 0.46              |
| 23:DB:1946:U:C2   | 23:DB:1947:C:C5    | 3.03                     | 0.46              |
| 23:DB:2090:A:H2'  | 46:DZ:49:ARG:CZ    | 2.45                     | 0.46              |
| 23:DB:2228:G:H2'  | 23:DB:2229:U:H6    | 1.77                     | 0.46              |
| 23:DB:2502:G:H5'  | 23:DB:2503:A:C5'   | 2.36                     | 0.46              |
| 23:DB:2515:C:H2'  | 23:DB:2516:A:H8    | 1.81                     | 0.46              |
| 23:DB:2700:A:H2'  | 23:DB:2701:U:C6    | 2.51                     | 0.46              |
| 23:DB:2896:C:H2'  | 23:DB:2897:U:H6    | 1.80                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:DD:168:GLU:CD  | 26:DD:168:GLU:H   | 2.23                     | 0.46              |
| 30:DH:83:LYS:O    | 30:DH:90:LEU:HA   | 2.14                     | 0.46              |
| 33:DL:89:VAL:O    | 33:DL:89:VAL:HG13 | 2.16                     | 0.46              |
| 35:DN:8:ARG:HD2   | 35:DN:46:ARG:CZ   | 2.44                     | 0.46              |
| 36:DO:21:LEU:CD2  | 36:DO:22:GLY:H    | 2.23                     | 0.46              |
| 37:DP:4:ILE:HG22  | 37:DP:4:ILE:O     | 2.15                     | 0.46              |
| 37:DP:26:GLU:O    | 37:DP:27:VAL:C    | 2.59                     | 0.46              |
| 37:DP:54:LEU:N    | 37:DP:58:PHE:HD1  | 2.13                     | 0.46              |
| 38:DQ:92:LYS:C    | 38:DQ:94:LEU:N    | 2.73                     | 0.46              |
| 39:DR:58:VAL:O    | 39:DR:58:VAL:HG13 | 2.14                     | 0.46              |
| 40:DS:41:LYS:HG2  | 40:DS:43:ALA:HB3  | 1.97                     | 0.46              |
| 43:DW:33:GLY:O    | 43:DW:66:VAL:HG23 | 2.15                     | 0.46              |
| 44:DX:4:LYS:HG3   | 44:DX:7:ARG:HE    | 1.81                     | 0.46              |
| 45:DY:2:LYS:N     | 45:DY:37:ARG:HB2  | 2.30                     | 0.46              |
| 52:DI:45:THR:C    | 52:DI:48:ILE:HG22 | 2.40                     | 0.46              |
| 1:AA:252:U:H2'    | 1:AA:253:A:C8     | 2.50                     | 0.46              |
| 1:AA:279:A:H5'    | 1:AA:281:G:O4'    | 2.15                     | 0.46              |
| 1:AA:547:A:H4'    | 1:AA:548:G:O5'    | 2.16                     | 0.46              |
| 1:AA:598:U:H2'    | 1:AA:599:C:C6     | 2.51                     | 0.46              |
| 1:AA:611:C:H2'    | 1:AA:612:C:H6     | 1.80                     | 0.46              |
| 1:AA:924:C:H2'    | 1:AA:925:G:H8     | 1.81                     | 0.46              |
| 1:AA:1005:A:H3'   | 1:AA:1006:G:C8    | 2.48                     | 0.46              |
| 1:AA:1050:G:C2'   | 1:AA:1051:C:H5'   | 2.44                     | 0.46              |
| 1:AA:1184:G:C2    | 1:AA:1185:G:C8    | 3.03                     | 0.46              |
| 1:AA:1234:C:H2'   | 1:AA:1235:U:C6    | 2.50                     | 0.46              |
| 1:AA:1243:C:H2'   | 1:AA:1244:G:C8    | 2.51                     | 0.46              |
| 1:AA:1374:A:H4'   | 6:AG:30:MET:HE1   | 1.97                     | 0.46              |
| 6:AG:91:ARG:HD3   | 6:AG:91:ARG:H     | 1.80                     | 0.46              |
| 6:AG:142:ARG:C    | 6:AG:146:ALA:HB3  | 2.41                     | 0.46              |
| 8:AI:18:VAL:HG21  | 8:AI:82:ILE:CG1   | 2.45                     | 0.46              |
| 8:AI:93:LEU:C     | 8:AI:93:LEU:HD12  | 2.40                     | 0.46              |
| 12:AM:3:ILE:HA    | 12:AM:56:ARG:CG   | 2.41                     | 0.46              |
| 16:AQ:26:ARG:HE   | 16:AQ:39:ARG:NH1  | 2.14                     | 0.46              |
| 16:AQ:65:PRO:HA   | 16:AQ:71:SER:OG   | 2.15                     | 0.46              |
| 19:AT:60:GLN:NE2  | 19:AT:61:ALA:H    | 2.12                     | 0.46              |
| 19:AT:66:ILE:HG23 | 19:AT:70:LYS:CD   | 2.45                     | 0.46              |
| 20:AB:9:LEU:H     | 20:AB:9:LEU:CD1   | 2.27                     | 0.46              |
| 20:AB:61:SER:HA   | 20:AB:224:ARG:CA  | 2.43                     | 0.46              |
| 21:AU:16:ARG:C    | 21:AU:18:PHE:H    | 2.21                     | 0.46              |
| 23:BB:372:G:O2'   | 23:BB:373:U:P     | 2.73                     | 0.46              |
| 23:BB:633:A:H2'   | 23:BB:634:C:O4'   | 2.15                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:1179:G:O2'   | 23:BB:1180:U:H5'   | 2.16                     | 0.46              |
| 23:BB:1186:G:H2'   | 23:BB:1187:G:O4'   | 2.16                     | 0.46              |
| 23:BB:1541:C:H2'   | 23:BB:1542:U:C6    | 2.50                     | 0.46              |
| 23:BB:1666:G:C2'   | 23:BB:1667:G:H5'   | 2.45                     | 0.46              |
| 23:BB:1824:G:H2'   | 23:BB:1825:U:H6    | 1.81                     | 0.46              |
| 23:BB:1947:C:O2'   | 23:BB:1948:G:H5'   | 2.15                     | 0.46              |
| 23:BB:2199:A:H3'   | 23:BB:2200:C:H6    | 1.80                     | 0.46              |
| 23:BB:2317:A:N6    | 23:BB:2318:G:C4    | 2.83                     | 0.46              |
| 23:BB:2320:U:H3'   | 23:BB:2321:U:C5'   | 2.46                     | 0.46              |
| 23:BB:2627:G:O2'   | 23:BB:2781:A:N1    | 2.45                     | 0.46              |
| 23:BB:2714:G:H2'   | 23:BB:2715:C:H6    | 1.80                     | 0.46              |
| 25:BC:128:THR:HA   | 25:BC:190:THR:CA   | 2.40                     | 0.46              |
| 28:BF:161:SER:HB3  | 28:BF:164:GLU:HB2  | 1.97                     | 0.46              |
| 29:BG:17:LYS:O     | 29:BG:23:ILE:HD12  | 2.14                     | 0.46              |
| 30:BH:2:GLN:HE22   | 30:BH:19:VAL:C     | 2.23                     | 0.46              |
| 31:BJ:98:GLU:O     | 31:BJ:100:VAL:N    | 2.48                     | 0.46              |
| 33:BL:78:ARG:NH2   | 33:BL:110:VAL:HG11 | 2.30                     | 0.46              |
| 34:BM:8:LYS:CE     | 34:BM:70:ASP:HA    | 2.44                     | 0.46              |
| 36:BO:9:ARG:HG3    | 36:BO:12:THR:HG21  | 1.97                     | 0.46              |
| 36:BO:16:ARG:CD    | 36:BO:20:GLU:HG3   | 2.45                     | 0.46              |
| 39:BR:5:PHE:CG     | 39:BR:6:GLN:N      | 2.84                     | 0.46              |
| 40:BS:103:ILE:HG23 | 40:BS:104:THR:N    | 2.29                     | 0.46              |
| 41:BT:12:ARG:HH21  | 44:BX:29:ARG:CZ    | 2.28                     | 0.46              |
| 48:B1:49:LYS:N     | 48:B1:49:LYS:HD2   | 2.30                     | 0.46              |
| 52:BI:135:MET:HE2  | 52:BI:137:LEU:HD11 | 1.97                     | 0.46              |
| 1:CA:49:U:O2'      | 1:CA:50:A:H2'      | 2.14                     | 0.46              |
| 1:CA:60:A:C4'      | 1:CA:61:G:O5'      | 2.63                     | 0.46              |
| 1:CA:484:G:O2'     | 1:CA:485:U:OP2     | 2.28                     | 0.46              |
| 1:CA:633:G:H2'     | 1:CA:634:C:H6      | 1.81                     | 0.46              |
| 1:CA:699:C:C3'     | 1:CA:700:G:H5''    | 2.44                     | 0.46              |
| 1:CA:754:C:H3'     | 1:CA:754:C:O2      | 2.15                     | 0.46              |
| 1:CA:836:G:O2'     | 1:CA:837:U:H5'     | 2.15                     | 0.46              |
| 1:CA:1342:C:H4'    | 8:CI:126:PHE:O     | 2.15                     | 0.46              |
| 2:CC:86:LEU:O      | 2:CC:89:VAL:HG22   | 2.14                     | 0.46              |
| 4:CE:43:GLY:O      | 4:CE:72:ASN:HA     | 2.15                     | 0.46              |
| 4:CE:110:MET:HE1   | 4:CE:124:ALA:HB1   | 1.98                     | 0.46              |
| 7:CH:74:ILE:O      | 7:CH:74:ILE:HG23   | 2.15                     | 0.46              |
| 8:CI:108:ARG:O     | 8:CI:108:ARG:HG3   | 2.15                     | 0.46              |
| 10:CK:30:ILE:C     | 10:CK:30:ILE:HD12  | 2.40                     | 0.46              |
| 10:CK:110:THR:HB   | 21:CU:3:ILE:O      | 2.15                     | 0.46              |
| 12:CM:47:LEU:HD12  | 12:CM:51:GLN:HB2   | 1.98                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 20:CB:63:LYS:HD2   | 20:CB:87:ASP:OD2  | 2.14                     | 0.46              |
| 23:DB:27:G:H1'     | 23:DB:513:A:N6    | 2.30                     | 0.46              |
| 23:DB:39:G:H2'     | 23:DB:40:U:H6     | 1.80                     | 0.46              |
| 23:DB:131:A:H2'    | 23:DB:132:G:C8    | 2.48                     | 0.46              |
| 23:DB:533:G:N2     | 38:DQ:40:LYS:HD2  | 2.30                     | 0.46              |
| 23:DB:1328:A:H2'   | 23:DB:1330:C:C4   | 2.50                     | 0.46              |
| 23:DB:1450:G:N2    | 23:DB:1452:G:H1   | 1.95                     | 0.46              |
| 23:DB:1526:C:H2'   | 23:DB:1527:G:O4'  | 2.14                     | 0.46              |
| 23:DB:1707:G:H2'   | 23:DB:1708:C:H6   | 1.80                     | 0.46              |
| 23:DB:1947:C:O2'   | 23:DB:1948:G:H5'  | 2.15                     | 0.46              |
| 23:DB:2025:C:H2'   | 23:DB:2026:U:H6   | 1.77                     | 0.46              |
| 23:DB:2299:U:H2'   | 23:DB:2300:C:H6   | 1.80                     | 0.46              |
| 23:DB:2529:G:C4'   | 29:DG:175:LYS:HD3 | 2.46                     | 0.46              |
| 23:DB:2800:A:C4    | 23:DB:2801:G:H1'  | 2.51                     | 0.46              |
| 25:DC:28:PRO:CG    | 25:DC:79:ARG:NE   | 2.76                     | 0.46              |
| 25:DC:58:LYS:HG3   | 25:DC:58:LYS:O    | 2.15                     | 0.46              |
| 25:DC:243:PRO:CB   | 25:DC:248:GLY:HA2 | 2.46                     | 0.46              |
| 26:DD:118:PHE:HA   | 26:DD:164:GLN:HG2 | 1.96                     | 0.46              |
| 27:DE:143:LEU:HD13 | 27:DE:185:LYS:HZ2 | 1.80                     | 0.46              |
| 27:DE:161:ALA:HB1  | 27:DE:168:ASP:O   | 2.15                     | 0.46              |
| 27:DE:184:ASP:HB3  | 33:DL:13:LYS:HE3  | 1.97                     | 0.46              |
| 27:DE:189:THR:C    | 27:DE:191:ASP:N   | 2.72                     | 0.46              |
| 28:DF:69:ALA:HB3   | 28:DF:81:GLY:H    | 1.81                     | 0.46              |
| 31:DJ:76:HIS:HB2   | 31:DJ:86:GLN:CD   | 2.41                     | 0.46              |
| 33:DL:63:LYS:HB2   | 50:D3:26:ALA:CB   | 2.43                     | 0.46              |
| 34:DM:62:LYS:N     | 34:DM:104:GLU:HB3 | 2.20                     | 0.46              |
| 36:DO:31:THR:HG22  | 36:DO:33:ARG:H    | 1.79                     | 0.46              |
| 38:DQ:39:ILE:HG13  | 38:DQ:40:LYS:H    | 1.79                     | 0.46              |
| 42:DU:43:LYS:HB2   | 42:DU:43:LYS:NZ   | 2.30                     | 0.46              |
| 50:D3:12:ARG:CD    | 50:D3:23:HIS:HB2  | 2.45                     | 0.46              |
| 52:DI:16:MET:N     | 52:DI:42:ASN:OD1  | 2.49                     | 0.46              |
| 1:AA:619:U:O2      | 3:AD:129:VAL:HG13 | 2.15                     | 0.46              |
| 1:AA:1180:A:P      | 8:AI:98:ARG:HH22  | 2.38                     | 0.46              |
| 1:AA:1201:A:C1'    | 1:AA:1202:U:OP2   | 2.58                     | 0.46              |
| 1:AA:1332:A:H2'    | 1:AA:1333:A:H8    | 1.79                     | 0.46              |
| 1:AA:1382:C:H4'    | 6:AG:78:ARG:HD2   | 1.97                     | 0.46              |
| 2:AC:39:ARG:NH1    | 13:AN:91:GLU:HG2  | 2.31                     | 0.46              |
| 2:AC:59:PRO:HD2    | 2:AC:62:SER:O     | 2.15                     | 0.46              |
| 3:AD:2:ARG:O       | 3:AD:3:TYR:HB2    | 2.15                     | 0.46              |
| 5:AF:6:ILE:HD12    | 5:AF:88:MET:O     | 2.15                     | 0.46              |
| 6:AG:125:ASP:HB3   | 6:AG:130:LYS:CB   | 2.35                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:AI:40:ARG:HA     | 8:AI:44:ARG:HH21   | 1.81                     | 0.46              |
| 8:AI:112:ARG:HH11  | 8:AI:112:ARG:CB    | 2.27                     | 0.46              |
| 10:AK:41:LEU:HB3   | 10:AK:76:TYR:HE1   | 1.81                     | 0.46              |
| 10:AK:56:LYS:O     | 10:AK:58:THR:N     | 2.49                     | 0.46              |
| 11:AL:86:VAL:HG11  | 11:AL:89:LEU:HD23  | 1.97                     | 0.46              |
| 16:AQ:10:ARG:O     | 16:AQ:22:VAL:HG13  | 2.15                     | 0.46              |
| 20:AB:95:TRP:CH2   | 20:AB:100:LEU:HB2  | 2.50                     | 0.46              |
| 20:AB:100:LEU:O    | 20:AB:178:LEU:HG   | 2.16                     | 0.46              |
| 21:AU:20:ARG:CA    | 21:AU:24:LYS:HG3   | 2.39                     | 0.46              |
| 23:BB:425:G:H2'    | 23:BB:426:C:C6     | 2.50                     | 0.46              |
| 23:BB:857:G:H5'    | 43:BW:55:ASP:OD2   | 2.15                     | 0.46              |
| 23:BB:1154:G:OP2   | 38:BQ:57:ARG:NH1   | 2.49                     | 0.46              |
| 23:BB:1623:G:O2'   | 23:BB:1624:U:H5'   | 2.15                     | 0.46              |
| 23:BB:1666:G:O2'   | 23:BB:1667:G:H5'   | 2.14                     | 0.46              |
| 23:BB:2699:C:O2'   | 23:BB:2700:A:H5'   | 2.16                     | 0.46              |
| 24:BV:82:TYR:CD1   | 34:BM:36:VAL:HB    | 2.51                     | 0.46              |
| 25:BC:155:ARG:O    | 25:BC:157:ALA:N    | 2.48                     | 0.46              |
| 25:BC:243:PRO:HB2  | 25:BC:248:GLY:H    | 1.81                     | 0.46              |
| 27:BE:177:PRO:HA   | 27:BE:180:LEU:HD12 | 1.95                     | 0.46              |
| 31:BJ:45:THR:HB    | 38:BQ:63:ARG:NH1   | 2.30                     | 0.46              |
| 33:BL:63:LYS:HB2   | 50:B3:11:LYS:HZ2   | 1.80                     | 0.46              |
| 33:BL:73:ILE:O     | 33:BL:74:THR:C     | 2.59                     | 0.46              |
| 34:BM:82:MET:HB2   | 34:BM:84:LYS:CE    | 2.45                     | 0.46              |
| 34:BM:124:LEU:N    | 34:BM:124:LEU:HD23 | 2.31                     | 0.46              |
| 36:BO:45:SER:C     | 36:BO:47:VAL:N     | 2.73                     | 0.46              |
| 41:BT:28:ASN:N     | 41:BT:28:ASN:ND2   | 2.62                     | 0.46              |
| 46:BZ:59:ARG:HH21  | 46:BZ:62:LYS:HZ2   | 1.61                     | 0.46              |
| 49:B2:30:VAL:O     | 49:B2:33:ARG:HG3   | 2.15                     | 0.46              |
| 52:BI:35:MET:SD    | 52:BI:35:MET:C     | 2.98                     | 0.46              |
| 52:BI:64:ARG:C     | 52:BI:64:ARG:HD2   | 2.39                     | 0.46              |
| 1:CA:336:A:O2'     | 1:CA:337:G:H5'     | 2.15                     | 0.46              |
| 1:CA:409:U:OP1     | 3:CD:23:GLY:HA3    | 2.15                     | 0.46              |
| 1:CA:546:A:OP1     | 3:CD:69:ARG:HB2    | 2.15                     | 0.46              |
| 1:CA:691:G:H2'     | 1:CA:692:U:C6      | 2.51                     | 0.46              |
| 1:CA:1190:G:P      | 2:CC:4:VAL:HG12    | 2.56                     | 0.46              |
| 1:CA:1434:A:H2'    | 1:CA:1435:G:C8     | 2.50                     | 0.46              |
| 6:CG:65:LEU:C      | 6:CG:67:ASN:H      | 2.23                     | 0.46              |
| 6:CG:78:ARG:HH11   | 6:CG:81:GLY:N      | 2.12                     | 0.46              |
| 11:CL:30:ARG:HG2   | 11:CL:31:GLY:N     | 2.30                     | 0.46              |
| 12:CM:106:ARG:HH11 | 12:CM:106:ARG:CA   | 2.28                     | 0.46              |
| 19:CT:69:ASN:H     | 19:CT:69:ASN:HD22  | 1.60                     | 0.46              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DB:138:U:H2'   | 23:DB:140:C:N1    | 2.30                     | 0.46              |
| 23:DB:870:U:O2'   | 23:DB:871:U:H5'   | 2.15                     | 0.46              |
| 23:DB:988:A:OP1   | 45:DY:10:ARG:HB3  | 2.15                     | 0.46              |
| 23:DB:1940:U:H1'  | 23:DB:1941:C:H5   | 1.81                     | 0.46              |
| 23:DB:2616:C:H2'  | 23:DB:2617:U:H6   | 1.81                     | 0.46              |
| 23:DB:2648:G:H2'  | 23:DB:2649:C:H6   | 1.80                     | 0.46              |
| 23:DB:2699:C:O2'  | 23:DB:2700:A:H5'  | 2.15                     | 0.46              |
| 55:DB:3213:HOH:O  | 33:DL:41:ARG:HB2  | 2.14                     | 0.46              |
| 34:DM:14:LYS:HB3  | 34:DM:72:PRO:HG3  | 1.97                     | 0.46              |
| 38:DQ:52:ARG:CG   | 38:DQ:53:LYS:N    | 2.79                     | 0.46              |
| 43:DW:82:GLU:HG3  | 43:DW:83:ALA:N    | 2.29                     | 0.46              |
| 46:DZ:54:GLY:O    | 46:DZ:57:VAL:HB   | 2.15                     | 0.46              |
| 51:D4:15:LYS:HE3  | 51:D4:15:LYS:HB2  | 1.79                     | 0.46              |
| 52:DI:78:LEU:HA   | 52:DI:81:LYS:HE2  | 1.98                     | 0.46              |
| 1:AA:512:U:H2'    | 1:AA:513:C:C6     | 2.49                     | 0.46              |
| 1:AA:633:G:H2'    | 1:AA:634:C:H6     | 1.80                     | 0.46              |
| 1:AA:812:G:OP1    | 1:AA:812:G:H4'    | 2.16                     | 0.46              |
| 1:AA:1016:A:H5'   | 1:AA:1218:C:H4'   | 1.98                     | 0.46              |
| 1:AA:1149:C:O2'   | 1:AA:1150:A:H5'   | 2.15                     | 0.46              |
| 1:AA:1181:G:O4'   | 1:AA:1181:G:OP2   | 2.33                     | 0.46              |
| 1:AA:1462:C:H2'   | 1:AA:1463:U:C6    | 2.50                     | 0.46              |
| 5:AF:32:ALA:HB1   | 5:AF:70:VAL:HG11  | 1.97                     | 0.46              |
| 6:AG:41:ILE:CD1   | 6:AG:116:ALA:HB2  | 2.46                     | 0.46              |
| 10:AK:80:ASN:OD1  | 10:AK:105:ARG:HB3 | 2.15                     | 0.46              |
| 10:AK:125:LYS:O   | 10:AK:126:ARG:O   | 2.33                     | 0.46              |
| 22:BA:18:G:H2'    | 22:BA:19:C:H6     | 1.81                     | 0.46              |
| 23:BB:169:G:O2'   | 23:BB:170:U:H5'   | 2.15                     | 0.46              |
| 23:BB:692:C:H2'   | 23:BB:693:A:H8    | 1.80                     | 0.46              |
| 23:BB:811:U:OP2   | 33:BL:31:GLY:HA2  | 2.16                     | 0.46              |
| 23:BB:1252:G:H22  | 38:BQ:36:GLN:NE2  | 2.14                     | 0.46              |
| 23:BB:1368:G:H5'  | 49:B2:25:LYS:HD3  | 1.98                     | 0.46              |
| 23:BB:1683:U:H2'  | 23:BB:1684:G:H8   | 1.80                     | 0.46              |
| 23:BB:1791:A:N1   | 23:BB:1829:A:H5'  | 2.30                     | 0.46              |
| 23:BB:1824:G:H2'  | 23:BB:1825:U:C6   | 2.50                     | 0.46              |
| 23:BB:2515:C:H2'  | 23:BB:2516:A:H8   | 1.81                     | 0.46              |
| 23:BB:2637:U:C2'  | 23:BB:2638:G:H5'  | 2.45                     | 0.46              |
| 23:BB:2716:C:O2'  | 23:BB:2717:C:H5'  | 2.16                     | 0.46              |
| 25:BC:141:HIS:HB3 | 25:BC:190:THR:HB  | 1.97                     | 0.46              |
| 25:BC:257:ARG:O   | 25:BC:261:ARG:NH1 | 2.49                     | 0.46              |
| 26:BD:103:ASP:C   | 26:BD:105:LYS:H   | 2.23                     | 0.46              |
| 27:BE:27:LEU:HD21 | 27:BE:100:MET:HG2 | 1.96                     | 0.46              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BE:102:ARG:O   | 27:BE:105:LEU:HG   | 2.15                     | 0.46              |
| 28:BF:165:GLY:HA2 | 28:BF:168:LEU:CD2  | 2.45                     | 0.46              |
| 28:BF:177:ARG:C   | 28:BF:177:ARG:NE   | 2.74                     | 0.46              |
| 29:BG:129:GLU:C   | 29:BG:130:ILE:HD12 | 2.40                     | 0.46              |
| 30:BH:53:GLU:C    | 30:BH:54:LEU:HD22  | 2.41                     | 0.46              |
| 30:BH:75:LEU:HD23 | 30:BH:76:GLU:N     | 2.31                     | 0.46              |
| 30:BH:89:LYS:HE2  | 30:BH:89:LYS:CA    | 2.46                     | 0.46              |
| 33:BL:59:ARG:NH1  | 50:B3:51:LYS:HB2   | 2.31                     | 0.46              |
| 33:BL:120:VAL:O   | 33:BL:120:VAL:HG13 | 2.16                     | 0.46              |
| 35:BN:13:ASN:C    | 35:BN:15:SER:N     | 2.74                     | 0.46              |
| 36:BO:19:GLN:HE21 | 43:BW:43:LYS:HE3   | 1.80                     | 0.46              |
| 39:BR:40:MET:C    | 39:BR:54:VAL:HG11  | 2.41                     | 0.46              |
| 39:BR:70:GLU:O    | 39:BR:71:LYS:HB2   | 2.14                     | 0.46              |
| 39:BR:82:HIS:ND1  | 39:BR:82:HIS:O     | 2.49                     | 0.46              |
| 41:BT:23:ALA:O    | 41:BT:24:MET:HE3   | 2.14                     | 0.46              |
| 42:BU:29:SER:O    | 42:BU:30:SER:HB2   | 2.16                     | 0.46              |
| 43:BW:75:ASN:HB3  | 43:BW:76:ARG:H     | 1.62                     | 0.46              |
| 46:BZ:5:ILE:CG2   | 46:BZ:63:ARG:HE    | 2.27                     | 0.46              |
| 48:B1:10:LEU:HD22 | 48:B1:25:ASN:ND2   | 2.31                     | 0.46              |
| 1:CA:148:G:N3     | 1:CA:1446:A:H2     | 2.13                     | 0.46              |
| 1:CA:691:G:H1'    | 1:CA:696:A:N6      | 2.30                     | 0.46              |
| 1:CA:768:A:H5'    | 1:CA:1524:C:H1'    | 1.97                     | 0.46              |
| 1:CA:812:G:H4'    | 1:CA:812:G:OP1     | 2.16                     | 0.46              |
| 1:CA:824:G:O2'    | 1:CA:825:A:H5'     | 2.14                     | 0.46              |
| 1:CA:1349:A:H2'   | 1:CA:1350:A:O4'    | 2.15                     | 0.46              |
| 1:CA:1473:G:O2'   | 1:CA:1474:U:H5'    | 2.16                     | 0.46              |
| 2:CC:76:ILE:O     | 2:CC:83:VAL:HG23   | 2.15                     | 0.46              |
| 2:CC:110:LEU:HD23 | 2:CC:110:LEU:N     | 2.29                     | 0.46              |
| 5:CF:92:THR:CG2   | 5:CF:93:LYS:H      | 2.28                     | 0.46              |
| 6:CG:71:THR:HA    | 6:CG:95:ARG:HE     | 1.81                     | 0.46              |
| 11:CL:86:VAL:HG22 | 11:CL:95:HIS:HE2   | 1.81                     | 0.46              |
| 12:CM:9:PRO:O     | 12:CM:44:ILE:HG12  | 2.15                     | 0.46              |
| 12:CM:10:ASP:HA   | 12:CM:44:ILE:CD1   | 2.46                     | 0.46              |
| 12:CM:63:VAL:O    | 12:CM:68:LEU:HD12  | 2.15                     | 0.46              |
| 13:CN:63:CYS:HB3  | 13:CN:68:ARG:N     | 2.23                     | 0.46              |
| 16:CQ:64:ARG:NH1  | 16:CQ:64:ARG:HB3   | 2.30                     | 0.46              |
| 20:CB:48:MET:HB3  | 20:CB:198:VAL:O    | 2.15                     | 0.46              |
| 20:CB:218:ALA:O   | 20:CB:221:ARG:HG2  | 2.16                     | 0.46              |
| 22:DA:38:C:H4'    | 36:DO:100:HIS:CE1  | 2.51                     | 0.46              |
| 23:DB:163:C:H2'   | 23:DB:164:C:O4'    | 2.15                     | 0.46              |
| 23:DB:231:A:H3'   | 23:DB:232:G:H8     | 1.81                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DB:322:A:C2    | 23:DB:340:A:C6    | 3.03                     | 0.46              |
| 23:DB:692:C:H2'   | 23:DB:693:A:C8    | 2.51                     | 0.46              |
| 23:DB:1042:G:H2'  | 23:DB:1043:C:H6   | 1.80                     | 0.46              |
| 23:DB:1192:G:O2'  | 23:DB:1193:G:H5'  | 2.16                     | 0.46              |
| 23:DB:1424:G:H2'  | 23:DB:1425:G:O4'  | 2.15                     | 0.46              |
| 23:DB:1487:U:H2'  | 23:DB:1488:C:C6   | 2.51                     | 0.46              |
| 23:DB:1623:G:O2'  | 23:DB:1624:U:H5'  | 2.15                     | 0.46              |
| 23:DB:1885:A:H3'  | 23:DB:1886:U:C6   | 2.51                     | 0.46              |
| 23:DB:2051:A:H4'  | 26:DD:145:SER:CB  | 2.44                     | 0.46              |
| 23:DB:2070:A:H2'  | 23:DB:2071:A:H8   | 1.80                     | 0.46              |
| 23:DB:2091:C:O4'  | 46:DZ:49:ARG:NE   | 2.49                     | 0.46              |
| 23:DB:2714:G:H2'  | 23:DB:2715:C:H6   | 1.80                     | 0.46              |
| 25:DC:243:PRO:HB3 | 25:DC:248:GLY:HA2 | 1.98                     | 0.46              |
| 25:DC:257:ARG:HG2 | 25:DC:257:ARG:NH1 | 2.31                     | 0.46              |
| 26:DD:36:GLN:HG2  | 26:DD:88:GLU:HA   | 1.97                     | 0.46              |
| 26:DD:62:LYS:HB2  | 26:DD:63:PRO:HD3  | 1.97                     | 0.46              |
| 28:DF:132:ARG:HD3 | 28:DF:133:GLU:N   | 2.25                     | 0.46              |
| 28:DF:141:ASP:O   | 28:DF:142:TYR:HB3 | 2.13                     | 0.46              |
| 29:DG:42:VAL:HB   | 29:DG:51:PHE:HA   | 1.96                     | 0.46              |
| 33:DL:39:LYS:HZ3  | 33:DL:39:LYS:CA   | 2.28                     | 0.46              |
| 33:DL:79:LEU:HG   | 33:DL:111:ILE:O   | 2.15                     | 0.46              |
| 34:DM:18:ARG:CD   | 34:DM:18:ARG:N    | 2.78                     | 0.46              |
| 34:DM:61:GLY:CA   | 34:DM:105:MET:HB2 | 2.45                     | 0.46              |
| 34:DM:73:ILE:HD11 | 34:DM:92:TRP:HE3  | 1.80                     | 0.46              |
| 34:DM:75:GLU:O    | 34:DM:86:LYS:HB3  | 2.15                     | 0.46              |
| 35:DN:4:ARG:HB3   | 35:DN:4:ARG:NH1   | 2.30                     | 0.46              |
| 39:DR:4:VAL:O     | 39:DR:41:ILE:HG12 | 2.15                     | 0.46              |
| 39:DR:76:LYS:O    | 39:DR:77:PHE:HB2  | 2.15                     | 0.46              |
| 48:D1:5:ARG:N     | 48:D1:27:ARG:HH22 | 2.12                     | 0.46              |
| 1:AA:529:G:H22    | 11:AL:47:ALA:HB2  | 1.80                     | 0.46              |
| 1:AA:834:U:H2'    | 1:AA:835:U:C6     | 2.50                     | 0.46              |
| 1:AA:840:C:N3     | 1:AA:842:U:H4'    | 2.30                     | 0.46              |
| 1:AA:1220:G:H4'   | 18:AS:33:TRP:O    | 2.16                     | 0.46              |
| 3:AD:54:LEU:HA    | 3:AD:202:LEU:HD22 | 1.97                     | 0.46              |
| 4:AE:41:GLY:HA2   | 4:AE:118:GLY:HA2  | 1.97                     | 0.46              |
| 4:AE:45:VAL:HG12  | 4:AE:116:VAL:HG23 | 1.98                     | 0.46              |
| 7:AH:51:GLU:O     | 7:AH:56:PRO:HA    | 2.15                     | 0.46              |
| 8:AI:46:VAL:HA    | 8:AI:49:GLN:HB2   | 1.98                     | 0.46              |
| 9:AJ:30:LYS:HG3   | 9:AJ:36:VAL:HB    | 1.98                     | 0.46              |
| 11:AL:27:PRO:HG2  | 11:AL:28:GLN:NE2  | 2.31                     | 0.46              |
| 20:AB:96:LEU:N    | 20:AB:99:MET:HE3  | 2.20                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:BA:117:G:OP1    | 36:BO:55:GLU:OE1  | 2.33                     | 0.46              |
| 23:BB:165:A:H2'    | 23:BB:166:U:H6    | 1.80                     | 0.46              |
| 23:BB:322:A:C2     | 23:BB:340:A:C6    | 3.03                     | 0.46              |
| 23:BB:459:U:H5'    | 49:B2:41:ARG:HH21 | 1.80                     | 0.46              |
| 23:BB:1453:A:N7    | 35:BN:72:ASP:OD1  | 2.49                     | 0.46              |
| 23:BB:1795:C:H2'   | 23:BB:1796:U:C6   | 2.51                     | 0.46              |
| 23:BB:1820:U:H3    | 25:BC:197:ALA:HA  | 1.79                     | 0.46              |
| 23:BB:2379:G:H2'   | 23:BB:2380:C:C6   | 2.51                     | 0.46              |
| 23:BB:2835:A:H61   | 23:BB:2878:U:H2'  | 1.81                     | 0.46              |
| 24:BV:44:HIS:O     | 24:BV:46:LYS:N    | 2.49                     | 0.46              |
| 25:BC:37:SER:H     | 25:BC:62:ARG:CB   | 2.29                     | 0.46              |
| 25:BC:59:GLN:O     | 25:BC:60:ALA:HB3  | 2.15                     | 0.46              |
| 25:BC:79:ARG:HH11  | 25:BC:80:LEU:N    | 2.11                     | 0.46              |
| 25:BC:209:ALA:C    | 25:BC:213:ARG:HD2 | 2.41                     | 0.46              |
| 25:BC:222:THR:C    | 25:BC:224:MET:N   | 2.73                     | 0.46              |
| 26:BD:114:LYS:HE3  | 26:BD:196:ALA:CB  | 2.45                     | 0.46              |
| 26:BD:159:LYS:C    | 26:BD:159:LYS:HD3 | 2.41                     | 0.46              |
| 26:BD:166:GLY:O    | 26:BD:167:ASN:C   | 2.58                     | 0.46              |
| 30:BH:3:VAL:CG2    | 30:BH:21:VAL:HG21 | 2.45                     | 0.46              |
| 31:BJ:80:HIS:O     | 31:BJ:81:ILE:C    | 2.59                     | 0.46              |
| 32:BK:2:ILE:HG22   | 32:BK:67:LYS:HZ1  | 1.81                     | 0.46              |
| 33:BL:63:LYS:CA    | 50:B3:24:LYS:HD3  | 2.46                     | 0.46              |
| 33:BL:83:ALA:O     | 33:BL:84:LYS:O    | 2.34                     | 0.46              |
| 34:BM:66:ARG:H     | 34:BM:100:LYS:HB2 | 1.80                     | 0.46              |
| 34:BM:108:VAL:HG23 | 34:BM:112:LEU:CD1 | 2.40                     | 0.46              |
| 35:BN:73:ASN:CA    | 35:BN:76:VAL:HG13 | 2.45                     | 0.46              |
| 36:BO:26:LEU:HD13  | 36:BO:92:PHE:O    | 2.16                     | 0.46              |
| 38:BQ:97:ILE:HA    | 38:BQ:100:PHE:CE2 | 2.51                     | 0.46              |
| 39:BR:79:ARG:HD3   | 39:BR:86:GLN:CD   | 2.40                     | 0.46              |
| 40:BS:34:ASP:CA    | 40:BS:37:THR:HG22 | 2.45                     | 0.46              |
| 40:BS:69:LEU:O     | 40:BS:110:ARG:HD2 | 2.15                     | 0.46              |
| 46:BZ:12:ILE:HG22  | 46:BZ:24:ILE:HD11 | 1.96                     | 0.46              |
| 50:B3:4:LYS:HE3    | 50:B3:58:ILE:HB   | 1.98                     | 0.46              |
| 51:B4:24:ARG:HD3   | 51:B4:26:ILE:HG23 | 1.98                     | 0.46              |
| 52:BI:102:ARG:HB2  | 52:BI:141:ASP:OD2 | 2.16                     | 0.46              |
| 52:BI:125:THR:O    | 52:BI:129:GLU:HG3 | 2.16                     | 0.46              |
| 1:CA:109:A:H4'     | 1:CA:110:C:OP2    | 2.16                     | 0.46              |
| 1:CA:455:G:H2'     | 1:CA:456:A:C8     | 2.51                     | 0.46              |
| 1:CA:782:A:H4'     | 1:CA:1514:G:O2'   | 2.16                     | 0.46              |
| 1:CA:1131:G:H2'    | 1:CA:1132:C:H5'   | 1.98                     | 0.46              |
| 1:CA:1411:C:O2'    | 1:CA:1412:C:H5'   | 2.15                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:1432:G:H1'    | 1:CA:1468:A:N6    | 2.31                     | 0.46              |
| 1:CA:1492:A:N6     | 1:CA:1494:G:N9    | 2.64                     | 0.46              |
| 1:CA:1505:G:N7     | 53:CA:1601:KSG:H3 | 2.31                     | 0.46              |
| 2:CC:55:VAL:HG23   | 2:CC:66:THR:HB    | 1.98                     | 0.46              |
| 2:CC:174:LEU:HD21  | 2:CC:200:TRP:CD1  | 2.51                     | 0.46              |
| 3:CD:155:LYS:C     | 3:CD:157:ALA:H    | 2.23                     | 0.46              |
| 3:CD:160:LEU:HD22  | 3:CD:160:LEU:C    | 2.41                     | 0.46              |
| 4:CE:95:MET:HG3    | 4:CE:124:ALA:CB   | 2.44                     | 0.46              |
| 6:CG:8:GLN:HE21    | 6:CG:8:GLN:HA     | 1.81                     | 0.46              |
| 8:CI:8:THR:OG1     | 8:CI:9:GLY:N      | 2.49                     | 0.46              |
| 13:CN:30:ILE:HB    | 13:CN:44:VAL:CB   | 2.44                     | 0.46              |
| 13:CN:76:PHE:O     | 13:CN:78:LEU:HD13 | 2.15                     | 0.46              |
| 16:CQ:63:CYS:SG    | 16:CQ:66:LEU:HD11 | 2.56                     | 0.46              |
| 20:CB:125:PHE:C    | 20:CB:127:LYS:H   | 2.23                     | 0.46              |
| 23:DB:458:G:C2'    | 23:DB:459:U:OP2   | 2.64                     | 0.46              |
| 23:DB:934:U:H2'    | 23:DB:935:C:H6    | 1.80                     | 0.46              |
| 23:DB:948:C:H2'    | 23:DB:949:G:H8    | 1.81                     | 0.46              |
| 23:DB:1750:G:H2'   | 23:DB:1751:U:C6   | 2.50                     | 0.46              |
| 23:DB:1827:U:O2'   | 23:DB:1828:G:H5'  | 2.14                     | 0.46              |
| 23:DB:1841:U:H2'   | 23:DB:1842:G:H8   | 1.79                     | 0.46              |
| 23:DB:2515:C:OP1   | 31:DJ:82:GLY:C    | 2.59                     | 0.46              |
| 23:DB:2581:G:OP1   | 26:DD:134:HIS:CD2 | 2.69                     | 0.46              |
| 24:DV:93:ARG:HG2   | 24:DV:94:ALA:N    | 2.30                     | 0.46              |
| 25:DC:51:ARG:NH1   | 25:DC:54:GLY:HA3  | 2.20                     | 0.46              |
| 26:DD:21:SER:O     | 26:DD:23:PRO:HD3  | 2.16                     | 0.46              |
| 27:DE:116:ASP:OD2  | 27:DE:185:LYS:HG3 | 2.16                     | 0.46              |
| 27:DE:148:ILE:HA   | 27:DE:185:LYS:CB  | 2.35                     | 0.46              |
| 30:DH:3:VAL:HG22   | 30:DH:21:VAL:CG1  | 2.28                     | 0.46              |
| 30:DH:124:THR:HG23 | 30:DH:128:HIS:CE1 | 2.49                     | 0.46              |
| 36:DO:55:GLU:O     | 36:DO:56:LYS:C    | 2.57                     | 0.46              |
| 38:DQ:39:ILE:CG1   | 38:DQ:40:LYS:N    | 2.79                     | 0.46              |
| 39:DR:41:ILE:HD12  | 39:DR:42:ALA:H    | 1.80                     | 0.46              |
| 39:DR:64:VAL:HG22  | 39:DR:65:ALA:N    | 2.23                     | 0.46              |
| 44:DX:28:LEU:HD13  | 44:DX:42:LEU:CG   | 2.45                     | 0.46              |
| 44:DX:31:GLN:O     | 44:DX:32:ALA:HB3  | 2.15                     | 0.46              |
| 48:D1:27:ARG:HG2   | 48:D1:27:ARG:O    | 2.15                     | 0.46              |
| 1:AA:328:C:H4'     | 1:AA:329:A:H5''   | 1.98                     | 0.46              |
| 1:AA:334:C:H2'     | 1:AA:335:C:H6     | 1.80                     | 0.46              |
| 1:AA:807:A:H2'     | 1:AA:808:C:C6     | 2.51                     | 0.46              |
| 1:AA:836:G:O2'     | 1:AA:837:U:H5'    | 2.15                     | 0.46              |
| 1:AA:920:U:H2'     | 1:AA:921:U:H6     | 1.81                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1010:U:H2'    | 1:AA:1011:C:C6     | 2.50                     | 0.46              |
| 1:AA:1310:G:O2'    | 1:AA:1311:A:H5'    | 2.15                     | 0.46              |
| 1:AA:1480:A:O2'    | 1:AA:1481:U:H5'    | 2.16                     | 0.46              |
| 3:AD:24:VAL:O      | 3:AD:25:ARG:HD2    | 2.15                     | 0.46              |
| 3:AD:131:ILE:O     | 3:AD:134:TYR:HB2   | 2.16                     | 0.46              |
| 4:AE:17:VAL:HA     | 4:AE:34:ALA:HA     | 1.98                     | 0.46              |
| 7:AH:93:LYS:HD3    | 7:AH:93:LYS:N      | 2.30                     | 0.46              |
| 9:AJ:39:PRO:HA     | 9:AJ:74:VAL:HG22   | 1.98                     | 0.46              |
| 11:AL:71:HIS:ND1   | 11:AL:72:ASN:N     | 2.63                     | 0.46              |
| 12:AM:1:ALA:O      | 12:AM:8:ILE:HG22   | 2.15                     | 0.46              |
| 23:BB:26:G:H2'     | 23:BB:27:G:O4'     | 2.15                     | 0.46              |
| 23:BB:144:A:O2'    | 23:BB:145:C:H5'    | 2.16                     | 0.46              |
| 23:BB:473:G:O2'    | 23:BB:474:G:H5'    | 2.15                     | 0.46              |
| 23:BB:494:G:O2'    | 23:BB:495:G:H5'    | 2.15                     | 0.46              |
| 23:BB:811:U:C4     | 33:BL:29:LYS:HD3   | 2.50                     | 0.46              |
| 23:BB:1021:A:N6    | 23:BB:1141:U:H3    | 1.98                     | 0.46              |
| 23:BB:1353:A:H2'   | 23:BB:1354:A:C8    | 2.50                     | 0.46              |
| 23:BB:2031:A:C6    | 23:BB:2498:C:H1'   | 2.50                     | 0.46              |
| 23:BB:2063:C:O2    | 23:BB:2450:A:N1    | 2.49                     | 0.46              |
| 23:BB:2336:A:HO2'  | 23:BB:2337:G:P     | 2.39                     | 0.46              |
| 23:BB:2393:U:OP1   | 50:B3:29:ARG:NE    | 2.49                     | 0.46              |
| 23:BB:2648:G:H2'   | 23:BB:2649:C:H6    | 1.80                     | 0.46              |
| 23:BB:2700:A:H2'   | 23:BB:2701:U:C6    | 2.51                     | 0.46              |
| 25:BC:78:GLU:CB    | 25:BC:92:LEU:HB3   | 2.46                     | 0.46              |
| 25:BC:127:ASN:ND2  | 25:BC:128:THR:N    | 2.55                     | 0.46              |
| 25:BC:136:VAL:CG1  | 25:BC:165:ALA:HA   | 2.39                     | 0.46              |
| 25:BC:212:TRP:C    | 25:BC:214:GLY:H    | 2.24                     | 0.46              |
| 25:BC:224:MET:N    | 25:BC:224:MET:SD   | 2.88                     | 0.46              |
| 26:BD:118:PHE:N    | 26:BD:164:GLN:HG3  | 2.31                     | 0.46              |
| 26:BD:170:VAL:HG11 | 26:BD:194:PRO:CG   | 2.46                     | 0.46              |
| 27:BE:18:THR:O     | 27:BE:19:PHE:C     | 2.58                     | 0.46              |
| 27:BE:52:VAL:C     | 27:BE:54:GLY:N     | 2.73                     | 0.46              |
| 27:BE:119:ILE:HA   | 27:BE:189:THR:H    | 1.81                     | 0.46              |
| 27:BE:153:LEU:H    | 27:BE:171:ASP:HB3  | 1.80                     | 0.46              |
| 27:BE:158:PHE:C    | 27:BE:160:ALA:H    | 2.22                     | 0.46              |
| 29:BG:32:LEU:HD21  | 29:BG:74:MET:CG    | 2.46                     | 0.46              |
| 30:BH:78:VAL:CG1   | 30:BH:102:ALA:HB1  | 2.46                     | 0.46              |
| 30:BH:78:VAL:HB    | 30:BH:143:ILE:O    | 2.16                     | 0.46              |
| 31:BJ:42:ALA:HB1   | 38:BQ:67:ALA:HB2   | 1.97                     | 0.46              |
| 33:BL:116:VAL:HG12 | 33:BL:117:THR:N    | 2.21                     | 0.46              |
| 35:BN:28:LEU:HD21  | 35:BN:113:ILE:HG21 | 1.96                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:BR:39:LEU:HA   | 39:BR:60:LYS:O    | 2.15                     | 0.46              |
| 42:BU:11:ILE:HB   | 42:BU:69:VAL:HG11 | 1.96                     | 0.46              |
| 43:BW:24:ARG:HG3  | 43:BW:59:PHE:HD1  | 1.81                     | 0.46              |
| 43:BW:56:HIS:HE1  | 43:BW:58:LEU:HB2  | 1.79                     | 0.46              |
| 1:CA:599:C:O2'    | 1:CA:600:A:H5'    | 2.15                     | 0.46              |
| 1:CA:628:G:H2'    | 1:CA:629:A:C8     | 2.51                     | 0.46              |
| 1:CA:737:C:H5'    | 5:CF:89:VAL:O     | 2.15                     | 0.46              |
| 1:CA:1006:G:H2'   | 1:CA:1007:U:H6    | 1.80                     | 0.46              |
| 1:CA:1347:G:O5'   | 8:CI:108:ARG:HB2  | 2.16                     | 0.46              |
| 1:CA:1349:A:OP1   | 8:CI:121:ARG:HB2  | 2.16                     | 0.46              |
| 1:CA:1422:G:H5''  | 32:DK:48:PRO:CB   | 2.39                     | 0.46              |
| 4:CE:154:ALA:HB1  | 7:CH:65:PHE:CZ    | 2.50                     | 0.46              |
| 7:CH:100:ILE:C    | 7:CH:100:ILE:HD12 | 2.41                     | 0.46              |
| 8:CI:9:GLY:O      | 8:CI:16:ALA:HB3   | 2.15                     | 0.46              |
| 8:CI:104:THR:HG22 | 8:CI:105:ARG:N    | 2.31                     | 0.46              |
| 10:CK:12:ARG:HD3  | 10:CK:13:LYS:NZ   | 2.29                     | 0.46              |
| 10:CK:70:ALA:HB1  | 10:CK:74:LYS:HB2  | 1.97                     | 0.46              |
| 12:CM:3:ILE:HA    | 12:CM:56:ARG:HH11 | 1.80                     | 0.46              |
| 12:CM:79:LEU:HA   | 12:CM:82:LEU:CG   | 2.46                     | 0.46              |
| 23:DB:307:G:N1    | 23:DB:310:A:OP2   | 2.48                     | 0.46              |
| 23:DB:834:G:H2'   | 23:DB:835:C:H6    | 1.80                     | 0.46              |
| 23:DB:1098:A:O3'  | 52:DI:4:VAL:O     | 2.33                     | 0.46              |
| 23:DB:1552:A:H2'  | 23:DB:1553:A:C5'  | 2.43                     | 0.46              |
| 23:DB:1759:A:H4'  | 23:DB:2715:C:O4'  | 2.16                     | 0.46              |
| 23:DB:1824:G:H2'  | 23:DB:1825:U:H6   | 1.80                     | 0.46              |
| 23:DB:1919:A:H2'  | 23:DB:1920:C:H5'  | 1.97                     | 0.46              |
| 23:DB:2208:C:H2'  | 23:DB:2209:G:C8   | 2.51                     | 0.46              |
| 23:DB:2311:A:O2'  | 28:DF:39:VAL:HG21 | 2.15                     | 0.46              |
| 23:DB:2386:A:H2'  | 23:DB:2387:U:H6   | 1.81                     | 0.46              |
| 23:DB:2543:G:H2'  | 23:DB:2544:G:C8   | 2.50                     | 0.46              |
| 23:DB:2645:G:H4'  | 23:DB:2732:G:H2'  | 1.96                     | 0.46              |
| 23:DB:2815:C:C2   | 23:DB:2816:G:C8   | 3.04                     | 0.46              |
| 23:DB:2816:G:N3   | 23:DB:2883:A:O2'  | 2.48                     | 0.46              |
| 26:DD:41:ALA:C    | 26:DD:43:ASP:H    | 2.23                     | 0.46              |
| 26:DD:146:ILE:N   | 26:DD:146:ILE:CD1 | 2.79                     | 0.46              |
| 27:DE:31:VAL:HG21 | 27:DE:104:ALA:CB  | 2.45                     | 0.46              |
| 28:DF:50:ASP:C    | 28:DF:52:ALA:H    | 2.22                     | 0.46              |
| 28:DF:100:GLU:C   | 28:DF:102:LEU:N   | 2.73                     | 0.46              |
| 34:DM:96:ILE:HG22 | 34:DM:97:GLN:OE1  | 2.16                     | 0.46              |
| 37:DP:91:VAL:HG23 | 37:DP:92:ARG:N    | 2.29                     | 0.46              |
| 39:DR:63:VAL:HG13 | 39:DR:64:VAL:N    | 2.30                     | 0.46              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:DR:81:LYS:O    | 39:DR:83:TYR:N    | 2.48                     | 0.46              |
| 40:DS:23:LEU:HD13 | 40:DS:25:ARG:NH2  | 2.22                     | 0.46              |
| 40:DS:23:LEU:HD23 | 47:D0:21:LEU:HD13 | 1.96                     | 0.46              |
| 41:DT:32:LEU:O    | 41:DT:83:ALA:HB3  | 2.15                     | 0.46              |
| 42:DU:42:LYS:H    | 42:DU:57:ILE:HG21 | 1.80                     | 0.46              |
| 43:DW:54:ARG:HD2  | 43:DW:54:ARG:N    | 2.31                     | 0.46              |
| 48:D1:47:ILE:O    | 48:D1:48:TYR:HB2  | 2.16                     | 0.46              |
| 49:D2:17:GLY:C    | 49:D2:18:PHE:CG   | 2.93                     | 0.46              |
| 52:DI:72:THR:OG1  | 52:DI:73:PRO:HD2  | 2.15                     | 0.46              |
| 1:AA:81:A:C2      | 1:AA:82:G:N7      | 2.83                     | 0.46              |
| 1:AA:239:U:H6     | 1:AA:239:U:H5'    | 1.80                     | 0.46              |
| 1:AA:285:C:H2'    | 1:AA:286:C:H6     | 1.81                     | 0.46              |
| 1:AA:1236:A:H2'   | 1:AA:1237:C:O4'   | 2.15                     | 0.46              |
| 5:AF:29:ILE:HD13  | 5:AF:64:VAL:CG1   | 2.45                     | 0.46              |
| 6:AG:94:ARG:CD    | 6:AG:98:LEU:HD11  | 2.43                     | 0.46              |
| 8:AI:51:LEU:HB3   | 8:AI:56:MET:CG    | 2.45                     | 0.46              |
| 10:AK:32:THR:HA   | 10:AK:43:TRP:HA   | 1.98                     | 0.46              |
| 10:AK:88:PRO:HA   | 10:AK:92:ARG:HD2  | 1.98                     | 0.46              |
| 11:AL:98:ARG:CB   | 11:AL:116:TYR:HA  | 2.45                     | 0.46              |
| 14:AO:15:GLY:C    | 14:AO:17:ASP:H    | 2.24                     | 0.46              |
| 18:AS:12:LEU:O    | 18:AS:15:LEU:HB3  | 2.15                     | 0.46              |
| 23:BB:30:G:O2'    | 23:BB:31:C:H5'    | 2.16                     | 0.46              |
| 23:BB:131:A:O2'   | 23:BB:132:G:H5'   | 2.15                     | 0.46              |
| 23:BB:215:G:H4'   | 23:BB:216:A:OP1   | 2.15                     | 0.46              |
| 23:BB:247:G:H4'   | 23:BB:386:G:C5    | 2.51                     | 0.46              |
| 23:BB:248:G:C2    | 23:BB:2431:U:H4'  | 2.51                     | 0.46              |
| 23:BB:527:C:O2'   | 23:BB:528:A:C8    | 2.66                     | 0.46              |
| 23:BB:615:U:O2    | 27:BE:38:GLY:HA3  | 2.15                     | 0.46              |
| 23:BB:682:G:H5'   | 49:B2:26:ASN:OD1  | 2.16                     | 0.46              |
| 23:BB:692:C:H2'   | 23:BB:693:A:C8    | 2.51                     | 0.46              |
| 23:BB:1113:U:H5'' | 29:BG:2:ARG:H     | 1.79                     | 0.46              |
| 23:BB:1747:U:H2'  | 23:BB:1748:C:H6   | 1.81                     | 0.46              |
| 23:BB:1791:A:C4'  | 25:BC:207:ALA:H   | 2.28                     | 0.46              |
| 23:BB:2239:G:H5'  | 25:BC:246:PRO:HG2 | 1.97                     | 0.46              |
| 23:BB:2297:A:N6   | 23:BB:2319:G:C5'  | 2.78                     | 0.46              |
| 24:BV:4:ILE:HD11  | 24:BV:61:LEU:CD1  | 2.46                     | 0.46              |
| 24:BV:77:VAL:HG21 | 24:BV:79:ARG:HH21 | 1.81                     | 0.46              |
| 26:BD:22:ILE:O    | 26:BD:22:ILE:HG12 | 2.15                     | 0.46              |
| 26:BD:38:LYS:N    | 26:BD:38:LYS:HD3  | 2.30                     | 0.46              |
| 27:BE:25:GLU:CD   | 33:BL:17:LYS:HG2  | 2.40                     | 0.46              |
| 27:BE:28:VAL:HG23 | 27:BE:29:HIS:N    | 2.31                     | 0.46              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BE:35:TYR:CE2  | 27:BE:178:VAL:HG21 | 2.50                     | 0.46              |
| 28:BF:133:GLU:CD  | 28:BF:150:GLY:H    | 2.24                     | 0.46              |
| 29:BG:6:ALA:N     | 29:BG:7:PRO:CD     | 2.79                     | 0.46              |
| 31:BJ:39:LYS:C    | 31:BJ:41:LYS:N     | 2.74                     | 0.46              |
| 32:BK:23:LYS:CG   | 32:BK:24:VAL:H     | 2.27                     | 0.46              |
| 32:BK:61:VAL:HG23 | 32:BK:85:VAL:HB    | 1.98                     | 0.46              |
| 33:BL:28:GLY:O    | 33:BL:29:LYS:HB2   | 2.15                     | 0.46              |
| 33:BL:88:GLY:O    | 33:BL:90:VAL:HG23  | 2.15                     | 0.46              |
| 35:BN:9:GLN:HE21  | 35:BN:17:ARG:NH2   | 2.14                     | 0.46              |
| 36:BO:15:ARG:HH22 | 36:BO:17:LYS:HD2   | 1.80                     | 0.46              |
| 38:BQ:89:ILE:O    | 38:BQ:89:ILE:HG12  | 2.15                     | 0.46              |
| 40:BS:51:LEU:HD13 | 40:BS:51:LEU:C     | 2.41                     | 0.46              |
| 51:B4:27:CYS:SG   | 51:B4:33:HIS:NE2   | 2.89                     | 0.46              |
| 1:CA:807:A:H2'    | 1:CA:808:C:C6      | 2.51                     | 0.46              |
| 1:CA:1095:U:H2'   | 1:CA:1096:C:H6     | 1.81                     | 0.46              |
| 1:CA:1388:C:H2'   | 1:CA:1389:C:H6     | 1.79                     | 0.46              |
| 1:CA:1486:G:H2'   | 1:CA:1487:G:C8     | 2.51                     | 0.46              |
| 2:CC:8:GLY:O      | 2:CC:11:LEU:HG     | 2.15                     | 0.46              |
| 2:CC:190:THR:HG22 | 2:CC:191:THR:H     | 1.80                     | 0.46              |
| 4:CE:87:VAL:O     | 4:CE:88:HIS:HB3    | 2.16                     | 0.46              |
| 7:CH:38:VAL:CG2   | 7:CH:111:THR:HG22  | 2.46                     | 0.46              |
| 9:CJ:73:LEU:HD13  | 9:CJ:73:LEU:C      | 2.41                     | 0.46              |
| 10:CK:92:ARG:HH11 | 10:CK:92:ARG:HG2   | 1.81                     | 0.46              |
| 11:CL:65:TYR:HB3  | 11:CL:95:HIS:CD2   | 2.51                     | 0.46              |
| 13:CN:45:LEU:O    | 13:CN:48:GLN:HG3   | 2.16                     | 0.46              |
| 15:CP:4:ILE:CD1   | 15:CP:57:ILE:HG12  | 2.44                     | 0.46              |
| 19:CT:69:ASN:ND2  | 19:CT:69:ASN:N     | 2.53                     | 0.46              |
| 20:CB:19:THR:HA   | 20:CB:37:VAL:HB    | 1.98                     | 0.46              |
| 21:CU:8:ASN:HB2   | 21:CU:9:GLU:OE2    | 2.16                     | 0.46              |
| 23:DB:6:A:H4'     | 31:DJ:133:ALA:C    | 2.41                     | 0.46              |
| 23:DB:242:G:O2'   | 23:DB:243:U:OP2    | 2.33                     | 0.46              |
| 23:DB:256:A:O2'   | 23:DB:257:C:H5'    | 2.16                     | 0.46              |
| 23:DB:277:G:H2'   | 23:DB:277:G:N3     | 2.31                     | 0.46              |
| 23:DB:479:A:O2'   | 23:DB:480:A:OP2    | 2.30                     | 0.46              |
| 23:DB:570:G:O2'   | 23:DB:571:U:H5'    | 2.16                     | 0.46              |
| 23:DB:964:C:O2'   | 23:DB:2273:A:H1'   | 2.15                     | 0.46              |
| 23:DB:1019:U:O2'  | 23:DB:1020:A:H5'   | 2.15                     | 0.46              |
| 23:DB:1108:U:H2'  | 23:DB:1109:C:H6    | 1.81                     | 0.46              |
| 23:DB:1163:G:O2'  | 23:DB:1164:C:H5'   | 2.16                     | 0.46              |
| 23:DB:1165:A:C2   | 23:DB:1166:G:N7    | 2.83                     | 0.46              |
| 23:DB:1537:G:H2'  | 23:DB:1538:G:O4'   | 2.14                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:1795:C:H2'  | 23:DB:1796:U:C6    | 2.51                     | 0.46              |
| 23:DB:2093:G:H2'  | 23:DB:2094:A:H8    | 1.81                     | 0.46              |
| 23:DB:2156:G:H2'  | 23:DB:2157:G:C4'   | 2.37                     | 0.46              |
| 23:DB:2373:G:H2'  | 23:DB:2374:C:H6    | 1.80                     | 0.46              |
| 23:DB:2415:G:H4'  | 33:DL:66:PHE:CB    | 2.46                     | 0.46              |
| 23:DB:2603:G:O2'  | 23:DB:2604:U:H5'   | 2.16                     | 0.46              |
| 23:DB:2722:G:H2'  | 23:DB:2723:C:H6    | 1.81                     | 0.46              |
| 27:DE:188:MET:CE  | 27:DE:190:ALA:HB2  | 2.46                     | 0.46              |
| 29:DG:12:ALA:C    | 29:DG:14:VAL:H     | 2.23                     | 0.46              |
| 29:DG:42:VAL:HA   | 29:DG:50:THR:O     | 2.16                     | 0.46              |
| 29:DG:94:ARG:H    | 29:DG:105:SER:HB2  | 1.80                     | 0.46              |
| 29:DG:132:LEU:C   | 29:DG:132:LEU:HD12 | 2.40                     | 0.46              |
| 30:DH:126:GLY:O   | 30:DH:145:ASN:HA   | 2.16                     | 0.46              |
| 32:DK:4:GLU:OE2   | 32:DK:23:LYS:HD2   | 2.15                     | 0.46              |
| 32:DK:84:CYS:O    | 32:DK:85:VAL:HB    | 2.16                     | 0.46              |
| 33:DL:92:LEU:HB2  | 33:DL:125:LEU:CD1  | 2.45                     | 0.46              |
| 35:DN:76:VAL:O    | 35:DN:80:PHE:HD1   | 1.98                     | 0.46              |
| 36:DO:100:HIS:HA  | 36:DO:104:GLN:NE2  | 2.30                     | 0.46              |
| 37:DP:52:ARG:HG2  | 37:DP:60:VAL:CG2   | 2.46                     | 0.46              |
| 38:DQ:52:ARG:HH11 | 38:DQ:52:ARG:HB3   | 1.79                     | 0.46              |
| 38:DQ:87:VAL:O    | 39:DR:54:VAL:HG21  | 2.16                     | 0.46              |
| 39:DR:79:ARG:HB3  | 39:DR:89:HIS:HE1   | 1.81                     | 0.46              |
| 42:DU:38:ILE:HG13 | 42:DU:62:ALA:CB    | 2.45                     | 0.46              |
| 42:DU:42:LYS:N    | 42:DU:57:ILE:HG21  | 2.31                     | 0.46              |
| 43:DW:44:PHE:CD2  | 43:DW:77:LYS:HB3   | 2.50                     | 0.46              |
| 43:DW:57:THR:HG22 | 43:DW:77:LYS:HG2   | 1.98                     | 0.46              |
| 49:D2:39:ARG:HG3  | 49:D2:39:ARG:HH11  | 1.79                     | 0.46              |
| 52:DI:18:ASN:N    | 52:DI:19:PRO:CD    | 2.78                     | 0.46              |
| 1:AA:28:A:O2'     | 1:AA:296:U:OP1     | 2.32                     | 0.46              |
| 1:AA:428:G:H4'    | 1:AA:429:U:O5'     | 2.16                     | 0.46              |
| 1:AA:628:G:H2'    | 1:AA:629:A:C8      | 2.51                     | 0.46              |
| 1:AA:820:U:H4'    | 1:AA:821:G:OP2     | 2.16                     | 0.46              |
| 1:AA:1202:U:H2'   | 1:AA:1203:C:C5'    | 2.46                     | 0.46              |
| 1:AA:1372:U:OP1   | 8:AI:72:SER:HB2    | 2.16                     | 0.46              |
| 2:AC:17:TRP:C     | 2:AC:19:SER:H      | 2.23                     | 0.46              |
| 2:AC:38:VAL:HG23  | 2:AC:39:ARG:N      | 2.29                     | 0.46              |
| 2:AC:111:ASP:O    | 2:AC:115:VAL:HG23  | 2.15                     | 0.46              |
| 3:AD:123:MET:HG3  | 3:AD:127:ARG:C     | 2.40                     | 0.46              |
| 9:AJ:15:HIS:CD2   | 9:AJ:19:ASP:HB2    | 2.51                     | 0.46              |
| 12:AM:58:GLU:HA   | 12:AM:61:LYS:HE2   | 1.98                     | 0.46              |
| 15:AP:44:SER:O    | 15:AP:45:GLU:C     | 2.59                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 20:AB:15:PHE:O     | 20:AB:40:ILE:HG13 | 2.16                     | 0.46              |
| 21:AU:15:LEU:O     | 21:AU:18:PHE:HB2  | 2.16                     | 0.46              |
| 23:BB:396:G:C4'    | 46:BZ:28:VAL:HG21 | 2.34                     | 0.46              |
| 23:BB:774:G:OP2    | 25:BC:47:ARG:HD3  | 2.15                     | 0.46              |
| 23:BB:788:A:H1'    | 49:B2:4:THR:OG1   | 2.15                     | 0.46              |
| 23:BB:1011:G:H5''  | 38:BQ:76:SER:OG   | 2.16                     | 0.46              |
| 23:BB:1083:U:C2    | 23:BB:1086:A:N1   | 2.83                     | 0.46              |
| 23:BB:1091:G:O2'   | 23:BB:1092:C:H5'  | 2.15                     | 0.46              |
| 23:BB:1712:U:H3'   | 23:BB:1713:A:C5'  | 2.46                     | 0.46              |
| 23:BB:1735:A:H2'   | 23:BB:1736:U:C6   | 2.50                     | 0.46              |
| 23:BB:1936:A:H2    | 23:BB:1943:U:C5   | 2.33                     | 0.46              |
| 23:BB:1946:U:C2    | 23:BB:1947:C:C5   | 3.03                     | 0.46              |
| 23:BB:2460:U:H2'   | 23:BB:2461:A:H8   | 1.81                     | 0.46              |
| 23:BB:2714:G:H2'   | 23:BB:2715:C:C6   | 2.51                     | 0.46              |
| 23:BB:2723:C:C5'   | 35:BN:3:HIS:HB2   | 2.46                     | 0.46              |
| 23:BB:2815:C:C2    | 23:BB:2816:G:C8   | 3.04                     | 0.46              |
| 23:BB:2816:G:N3    | 23:BB:2883:A:O2'  | 2.48                     | 0.46              |
| 25:BC:27:LYS:HG3   | 25:BC:80:LEU:HB2  | 1.96                     | 0.46              |
| 25:BC:62:ARG:NE    | 25:BC:62:ARG:O    | 2.48                     | 0.46              |
| 25:BC:115:ILE:HG23 | 25:BC:126:GLY:O   | 2.15                     | 0.46              |
| 26:BD:1:MET:CB     | 26:BD:84:LEU:HD22 | 2.40                     | 0.46              |
| 26:BD:23:PRO:HA    | 26:BD:190:LYS:HA  | 1.98                     | 0.46              |
| 26:BD:141:ARG:O    | 26:BD:142:VAL:C   | 2.58                     | 0.46              |
| 26:BD:148:GLN:HB3  | 26:BD:151:THR:CG2 | 2.45                     | 0.46              |
| 28:BF:35:LEU:O     | 28:BF:36:ASN:HB3  | 2.14                     | 0.46              |
| 29:BG:94:ARG:NH1   | 29:BG:127:GLN:HB2 | 2.31                     | 0.46              |
| 30:BH:3:VAL:HB     | 30:BH:37:VAL:CG2  | 2.46                     | 0.46              |
| 31:BJ:17:VAL:HG13  | 31:BJ:57:LEU:HD21 | 1.97                     | 0.46              |
| 32:BK:99:ILE:HD12  | 32:BK:99:ILE:N    | 2.30                     | 0.46              |
| 32:BK:99:ILE:CG2   | 32:BK:119:ALA:HB2 | 2.46                     | 0.46              |
| 33:BL:120:VAL:H    | 33:BL:138:ALA:CB  | 2.29                     | 0.46              |
| 35:BN:41:ALA:HB1   | 35:BN:97:ILE:HD12 | 1.97                     | 0.46              |
| 35:BN:78:LYS:O     | 35:BN:82:GLU:HB2  | 2.15                     | 0.46              |
| 36:BO:45:SER:C     | 36:BO:47:VAL:H    | 2.23                     | 0.46              |
| 36:BO:64:TYR:CD1   | 36:BO:74:VAL:HG21 | 2.50                     | 0.46              |
| 36:BO:84:GLU:OE1   | 36:BO:84:GLU:N    | 2.49                     | 0.46              |
| 38:BQ:5:ARG:CD     | 38:BQ:5:ARG:H     | 2.27                     | 0.46              |
| 39:BR:42:ALA:C     | 39:BR:44:GLY:H    | 2.23                     | 0.46              |
| 44:BX:30:MET:CG    | 44:BX:31:GLN:N    | 2.79                     | 0.46              |
| 47:B0:2:VAL:CG2    | 47:B0:3:GLN:N     | 2.79                     | 0.46              |
| 48:B1:10:LEU:HD22  | 48:B1:25:ASN:HD22 | 1.81                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 52:BI:46:ASP:HA   | 52:BI:50:LYS:HG3   | 1.96                     | 0.46              |
| 1:CA:278:G:H21    | 1:CA:279:A:N6      | 2.10                     | 0.46              |
| 1:CA:601:G:H2'    | 1:CA:602:A:H8      | 1.80                     | 0.46              |
| 1:CA:684:U:O2'    | 10:CK:39:ASN:HB3   | 2.16                     | 0.46              |
| 1:CA:721:G:H5''   | 17:CR:42:ARG:HH21  | 1.81                     | 0.46              |
| 2:CC:177:LEU:N    | 2:CC:177:LEU:HD22  | 2.31                     | 0.46              |
| 4:CE:76:ASN:O     | 4:CE:77:ASN:HB3    | 2.16                     | 0.46              |
| 8:CI:87:MET:HB2   | 8:CI:94:ARG:NH2    | 2.31                     | 0.46              |
| 8:CI:117:LEU:CD2  | 8:CI:123:ARG:HD3   | 2.46                     | 0.46              |
| 9:CJ:85:ASP:O     | 9:CJ:86:ALA:C      | 2.57                     | 0.46              |
| 11:CL:23:LEU:O    | 11:CL:25:ALA:N     | 2.49                     | 0.46              |
| 15:CP:28:ARG:C    | 15:CP:30:GLY:H     | 2.24                     | 0.46              |
| 18:CS:43:MET:O    | 18:CS:46:LEU:HB2   | 2.16                     | 0.46              |
| 22:DA:75:G:N1     | 22:DA:102:G:N2     | 2.64                     | 0.46              |
| 23:DB:139:U:H3'   | 23:DB:139:U:OP2    | 2.16                     | 0.46              |
| 23:DB:153:U:H2'   | 23:DB:154:U:O4'    | 2.16                     | 0.46              |
| 23:DB:267:C:H2'   | 23:DB:268:C:C6     | 2.50                     | 0.46              |
| 23:DB:443:A:N7    | 27:DE:40:ARG:HG2   | 2.31                     | 0.46              |
| 23:DB:814:C:OP1   | 39:DR:87:GLN:O     | 2.34                     | 0.46              |
| 23:DB:1162:G:O2'  | 23:DB:1163:G:H5'   | 2.16                     | 0.46              |
| 23:DB:1309:G:C5'  | 49:D2:7:PRO:HB2    | 2.46                     | 0.46              |
| 23:DB:1791:A:OP1  | 25:DC:211:ARG:HG2  | 2.16                     | 0.46              |
| 23:DB:2083:G:H2'  | 23:DB:2084:C:C6    | 2.51                     | 0.46              |
| 23:DB:2716:C:O2'  | 23:DB:2717:C:H5'   | 2.15                     | 0.46              |
| 23:DB:2721:A:H2'  | 23:DB:2722:G:C8    | 2.51                     | 0.46              |
| 23:DB:2800:A:N3   | 23:DB:2801:G:H1'   | 2.30                     | 0.46              |
| 25:DC:38:LYS:HG3  | 25:DC:39:SER:N     | 2.31                     | 0.46              |
| 25:DC:92:LEU:HD12 | 25:DC:101:ARG:O    | 2.16                     | 0.46              |
| 26:DD:28:GLU:CD   | 26:DD:97:SER:HA    | 2.41                     | 0.46              |
| 26:DD:29:VAL:CG2  | 26:DD:30:GLU:H     | 2.18                     | 0.46              |
| 26:DD:185:ASN:O   | 26:DD:186:LEU:HD12 | 2.16                     | 0.46              |
| 27:DE:154:ASP:OD2 | 27:DE:156:ASN:HB3  | 2.16                     | 0.46              |
| 28:DF:48:LEU:C    | 28:DF:50:ASP:H     | 2.24                     | 0.46              |
| 31:DJ:17:VAL:HA   | 31:DJ:55:ILE:HB    | 1.98                     | 0.46              |
| 32:DK:18:ARG:HB2  | 32:DK:45:GLU:HG2   | 1.98                     | 0.46              |
| 32:DK:43:ILE:HG22 | 32:DK:54:LYS:HA    | 1.97                     | 0.46              |
| 33:DL:62:PRO:HG3  | 50:D3:12:ARG:NH2   | 2.29                     | 0.46              |
| 33:DL:118:THR:O   | 33:DL:120:VAL:N    | 2.49                     | 0.46              |
| 34:DM:105:MET:O   | 34:DM:106:ASP:C    | 2.59                     | 0.46              |
| 36:DO:82:ALA:HB1  | 36:DO:87:ILE:CG2   | 2.46                     | 0.46              |
| 38:DQ:39:ILE:HA   | 38:DQ:43:GLN:NE2   | 2.30                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 38:DQ:53:LYS:HE2   | 38:DQ:53:LYS:N    | 2.13                     | 0.46              |
| 38:DQ:108:LEU:HA   | 38:DQ:111:LYS:CD  | 2.45                     | 0.46              |
| 39:DR:35:PHE:HB3   | 39:DR:64:VAL:HG12 | 1.97                     | 0.46              |
| 41:DT:35:ALA:O     | 41:DT:81:LYS:HD3  | 2.16                     | 0.46              |
| 43:DW:38:ARG:O     | 43:DW:39:GLN:HB3  | 2.15                     | 0.46              |
| 48:D1:49:LYS:HD2   | 48:D1:49:LYS:C    | 2.41                     | 0.46              |
| 52:DI:54:ILE:O     | 52:DI:54:ILE:HG23 | 2.16                     | 0.46              |
| 1:AA:41:G:H2'      | 1:AA:42:G:H8      | 1.81                     | 0.46              |
| 1:AA:82:G:C6       | 1:AA:88:U:O2      | 2.69                     | 0.46              |
| 1:AA:132:C:O2'     | 1:AA:133:U:H5'    | 2.15                     | 0.46              |
| 1:AA:382:A:O2'     | 1:AA:383:A:H5'    | 2.15                     | 0.46              |
| 1:AA:599:C:O2'     | 1:AA:600:A:H5'    | 2.15                     | 0.46              |
| 1:AA:601:G:H2'     | 1:AA:602:A:C8     | 2.50                     | 0.46              |
| 1:AA:1096:C:H2'    | 1:AA:1097:C:H6    | 1.81                     | 0.46              |
| 1:AA:1304:G:H2'    | 1:AA:1305:G:C1'   | 2.46                     | 0.46              |
| 1:AA:1427:C:O2'    | 1:AA:1428:A:H5'   | 2.16                     | 0.46              |
| 1:AA:1460:C:O2'    | 1:AA:1461:G:H5'   | 2.16                     | 0.46              |
| 3:AD:98:ASP:CB     | 3:AD:132:ALA:HB1  | 2.46                     | 0.46              |
| 4:AE:82:HIS:HB2    | 4:AE:83:PRO:HD2   | 1.98                     | 0.46              |
| 5:AF:50:PRO:HA     | 5:AF:54:LEU:O     | 2.16                     | 0.46              |
| 6:AG:11:ILE:HG12   | 6:AG:24:LYS:HE2   | 1.97                     | 0.46              |
| 7:AH:86:LYS:HB3    | 7:AH:90:GLU:HB2   | 1.97                     | 0.46              |
| 8:AI:119:LYS:HB3   | 8:AI:119:LYS:NZ   | 2.31                     | 0.46              |
| 10:AK:63:GLN:O     | 10:AK:67:GLU:HB3  | 2.15                     | 0.46              |
| 11:AL:35:ARG:O     | 11:AL:52:CYS:HB2  | 2.16                     | 0.46              |
| 11:AL:120:ARG:HH11 | 11:AL:120:ARG:HG3 | 1.81                     | 0.46              |
| 12:AM:21:ILE:C     | 12:AM:23:GLY:H    | 2.24                     | 0.46              |
| 15:AP:6:LEU:HD11   | 15:AP:71:VAL:HB   | 1.98                     | 0.46              |
| 18:AS:12:LEU:O     | 18:AS:12:LEU:HD23 | 2.15                     | 0.46              |
| 18:AS:29:PRO:HB3   | 18:AS:47:THR:CG2  | 2.46                     | 0.46              |
| 19:AT:60:GLN:HE21  | 19:AT:61:ALA:H    | 1.64                     | 0.46              |
| 23:BB:85:G:H5'     | 42:BU:28:LEU:CA   | 2.22                     | 0.46              |
| 23:BB:89:A:H2'     | 23:BB:90:U:C6     | 2.51                     | 0.46              |
| 23:BB:192:C:C2'    | 23:BB:193:U:H5'   | 2.43                     | 0.46              |
| 23:BB:441:U:H2'    | 23:BB:442:G:C8    | 2.49                     | 0.46              |
| 23:BB:523:C:O2'    | 23:BB:524:G:H5'   | 2.16                     | 0.46              |
| 23:BB:593:U:H2'    | 23:BB:594:U:H6    | 1.81                     | 0.46              |
| 23:BB:935:C:H2'    | 23:BB:936:A:H8    | 1.81                     | 0.46              |
| 23:BB:1313:U:O2    | 23:BB:1313:U:C2'  | 2.64                     | 0.46              |
| 23:BB:1408:G:H2'   | 23:BB:1409:U:H6   | 1.80                     | 0.46              |
| 23:BB:1553:A:O2'   | 23:BB:1554:U:H2'  | 2.16                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:1704:C:O2'   | 23:BB:1705:A:H5'   | 2.16                     | 0.46              |
| 23:BB:1979:U:C2'   | 23:BB:1980:G:H5'   | 2.46                     | 0.46              |
| 23:BB:1999:C:O2'   | 23:BB:2000:C:H5'   | 2.15                     | 0.46              |
| 23:BB:2014:A:P     | 40:BS:95:ARG:HH21  | 2.39                     | 0.46              |
| 23:BB:2280:G:O2'   | 23:BB:2388:A:N1    | 2.48                     | 0.46              |
| 23:BB:2307:G:O2'   | 23:BB:2311:A:N6    | 2.49                     | 0.46              |
| 23:BB:2334:U:OP2   | 36:BO:7:ARG:NE     | 2.49                     | 0.46              |
| 23:BB:2578:G:H1'   | 26:BD:145:SER:CB   | 2.46                     | 0.46              |
| 23:BB:2600:A:H62   | 25:BC:235:GLU:CB   | 2.29                     | 0.46              |
| 24:BV:70:ILE:HG12  | 24:BV:71:LYS:N     | 2.27                     | 0.46              |
| 25:BC:66:PHE:O     | 25:BC:68:ARG:HG3   | 2.16                     | 0.46              |
| 25:BC:77:VAL:HG21  | 25:BC:109:LEU:CG   | 2.43                     | 0.46              |
| 25:BC:185:ALA:C    | 25:BC:187:CYS:H    | 2.24                     | 0.46              |
| 26:BD:15:PHE:HB3   | 26:BD:18:ASP:CB    | 2.45                     | 0.46              |
| 26:BD:17:GLU:HA    | 37:BP:80:VAL:CG2   | 2.46                     | 0.46              |
| 26:BD:89:GLU:C     | 26:BD:91:THR:H     | 2.23                     | 0.46              |
| 26:BD:106:LYS:O    | 26:BD:206:ALA:HB2  | 2.16                     | 0.46              |
| 28:BF:56:LEU:HD23  | 28:BF:59:ILE:HG22  | 1.98                     | 0.46              |
| 28:BF:109:ARG:CB   | 28:BF:136:ILE:HG13 | 2.46                     | 0.46              |
| 28:BF:131:VAL:HG12 | 28:BF:132:ARG:N    | 2.30                     | 0.46              |
| 29:BG:34:ARG:HG3   | 29:BG:35:THR:N     | 2.30                     | 0.46              |
| 30:BH:27:ARG:HB2   | 30:BH:27:ARG:HH11  | 1.81                     | 0.46              |
| 31:BJ:7:LYS:HZ3    | 31:BJ:48:VAL:HB    | 1.81                     | 0.46              |
| 32:BK:58:LEU:HA    | 32:BK:89:ASN:HD22  | 1.80                     | 0.46              |
| 32:BK:91:SER:O     | 32:BK:92:GLU:C     | 2.59                     | 0.46              |
| 33:BL:94:THR:HG23  | 33:BL:95:LEU:H     | 1.80                     | 0.46              |
| 33:BL:103:ILE:HD13 | 33:BL:104:GLN:H    | 1.81                     | 0.46              |
| 34:BM:105:MET:HE3  | 34:BM:107:GLY:HA3  | 1.98                     | 0.46              |
| 35:BN:13:ASN:C     | 35:BN:15:SER:H     | 2.23                     | 0.46              |
| 36:BO:106:LEU:HD13 | 36:BO:106:LEU:O    | 2.16                     | 0.46              |
| 37:BP:109:ILE:O    | 37:BP:109:ILE:HG22 | 2.16                     | 0.46              |
| 40:BS:4:ILE:HD12   | 40:BS:106:VAL:HG22 | 1.98                     | 0.46              |
| 40:BS:8:ARG:O      | 40:BS:9:HIS:HB2    | 2.16                     | 0.46              |
| 40:BS:28:LYS:HB3   | 40:BS:71:VAL:HB    | 1.98                     | 0.46              |
| 42:BU:6:ARG:C      | 42:BU:8:ASP:N      | 2.73                     | 0.46              |
| 42:BU:66:VAL:O     | 42:BU:68:ASN:N     | 2.48                     | 0.46              |
| 42:BU:90:LYS:HD2   | 42:BU:91:LYS:H     | 1.81                     | 0.46              |
| 43:BW:43:LYS:HD2   | 43:BW:43:LYS:N     | 2.31                     | 0.46              |
| 46:BZ:7:PRO:O      | 46:BZ:8:LYS:HB3    | 2.16                     | 0.46              |
| 48:B1:46:VAL:C     | 48:B1:47:ILE:HG12  | 2.41                     | 0.46              |
| 52:BI:52:LEU:HD21  | 52:BI:81:LYS:NZ    | 2.31                     | 0.46              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:22:G:O2'      | 1:CA:23:C:H5'     | 2.16                     | 0.46              |
| 1:CA:132:C:O2'     | 1:CA:133:U:H5'    | 2.15                     | 0.46              |
| 1:CA:411:A:C5      | 1:CA:413:G:H1'    | 2.51                     | 0.46              |
| 1:CA:652:U:H1'     | 1:CA:653:U:C5     | 2.50                     | 0.46              |
| 1:CA:861:G:O2'     | 1:CA:862:C:H5'    | 2.15                     | 0.46              |
| 1:CA:932:C:H2'     | 1:CA:933:G:H8     | 1.80                     | 0.46              |
| 1:CA:956:U:H2'     | 1:CA:957:U:C6     | 2.50                     | 0.46              |
| 1:CA:1049:U:O2     | 1:CA:1049:U:H2'   | 2.14                     | 0.46              |
| 1:CA:1216:A:P      | 13:CN:2:LYS:HE2   | 2.56                     | 0.46              |
| 1:CA:1279:G:H22    | 9:CJ:45:ARG:HD2   | 1.80                     | 0.46              |
| 2:CC:143:LEU:HD13  | 2:CC:143:LEU:N    | 2.31                     | 0.46              |
| 4:CE:20:VAL:CG1    | 4:CE:31:SER:HB2   | 2.45                     | 0.46              |
| 8:CI:117:LEU:HD23  | 8:CI:123:ARG:HD3  | 1.97                     | 0.46              |
| 12:CM:52:ILE:O     | 12:CM:55:LEU:HB2  | 2.16                     | 0.46              |
| 14:CO:10:ILE:HD11  | 14:CO:29:ALA:CB   | 2.46                     | 0.46              |
| 14:CO:81:ILE:O     | 14:CO:85:GLY:N    | 2.48                     | 0.46              |
| 18:CS:14:LEU:HD12  | 18:CS:14:LEU:C    | 2.41                     | 0.46              |
| 18:CS:32:THR:HG22  | 18:CS:33:TRP:N    | 2.21                     | 0.46              |
| 20:CB:60:ALA:HA    | 20:CB:64:GLY:HA3  | 1.98                     | 0.46              |
| 20:CB:173:LYS:C    | 20:CB:173:LYS:HD2 | 2.41                     | 0.46              |
| 20:CB:195:VAL:HG12 | 20:CB:197:PHE:H   | 1.81                     | 0.46              |
| 23:DB:494:G:O2'    | 23:DB:495:G:H5'   | 2.16                     | 0.46              |
| 23:DB:741:U:H2'    | 23:DB:742:A:H8    | 1.79                     | 0.46              |
| 23:DB:1597:A:H5''  | 23:DB:1598:A:H5'  | 1.96                     | 0.46              |
| 23:DB:1665:A:O2'   | 23:DB:1666:G:H5'  | 2.15                     | 0.46              |
| 23:DB:2065:C:H5'   | 23:DB:2251:G:H21  | 1.81                     | 0.46              |
| 23:DB:2393:U:H5    | 50:D3:30:HIS:HE1  | 1.63                     | 0.46              |
| 23:DB:2393:U:O2'   | 23:DB:2394:C:H5'  | 2.15                     | 0.46              |
| 23:DB:2752:C:H2'   | 23:DB:2753:A:O4'  | 2.15                     | 0.46              |
| 23:DB:2776:A:H4'   | 23:DB:2777:G:C5'  | 2.46                     | 0.46              |
| 23:DB:2893:A:H4'   | 23:DB:2894:G:H5'  | 1.96                     | 0.46              |
| 26:DD:160:LYS:O    | 26:DD:161:MET:C   | 2.58                     | 0.46              |
| 31:DJ:28:LEU:O     | 31:DJ:28:LEU:HD22 | 2.16                     | 0.46              |
| 31:DJ:57:LEU:HG    | 31:DJ:128:ASN:HA  | 1.98                     | 0.46              |
| 33:DL:108:ALA:HB3  | 33:DL:125:LEU:HB2 | 1.98                     | 0.46              |
| 35:DN:33:ILE:HG12  | 35:DN:114:GLU:HB3 | 1.98                     | 0.46              |
| 35:DN:101:GLY:O    | 35:DN:102:PHE:HB3 | 2.16                     | 0.46              |
| 38:DQ:40:LYS:O     | 38:DQ:44:TYR:HB3  | 2.16                     | 0.46              |
| 38:DQ:57:ARG:NH2   | 38:DQ:92:LYS:HZ3  | 2.12                     | 0.46              |
| 40:DS:3:THR:HG21   | 40:DS:58:ALA:HB2  | 1.97                     | 0.46              |
| 40:DS:5:ALA:HB3    | 40:DS:54:ALA:HB2  | 1.98                     | 0.46              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:DT:47:VAL:HG22  | 41:DT:53:VAL:CG2   | 2.40                     | 0.46              |
| 42:DU:48:VAL:O     | 42:DU:48:VAL:HG12  | 2.16                     | 0.46              |
| 43:DW:55:ASP:CG    | 43:DW:56:HIS:N     | 2.74                     | 0.46              |
| 46:DZ:64:PHE:O     | 46:DZ:64:PHE:HD2   | 1.98                     | 0.46              |
| 48:D1:35:LEU:HD23  | 48:D1:35:LEU:N     | 2.31                     | 0.46              |
| 1:AA:109:A:H4'     | 1:AA:110:C:OP2     | 2.16                     | 0.45              |
| 1:AA:525:C:H2'     | 1:AA:526:C:C6      | 2.51                     | 0.45              |
| 1:AA:861:G:O2'     | 1:AA:862:C:H5'     | 2.15                     | 0.45              |
| 1:AA:955:U:O2'     | 1:AA:956:U:H5'     | 2.16                     | 0.45              |
| 1:AA:1098:C:C2'    | 1:AA:1099:G:H5'    | 2.46                     | 0.45              |
| 1:AA:1149:C:H2'    | 1:AA:1150:A:H8     | 1.80                     | 0.45              |
| 1:AA:1499:A:O2'    | 1:AA:1500:A:H5'    | 2.16                     | 0.45              |
| 3:AD:160:LEU:H     | 3:AD:160:LEU:CD1   | 2.22                     | 0.45              |
| 3:AD:169:TRP:CB    | 3:AD:183:ARG:HH21  | 2.30                     | 0.45              |
| 10:AK:57:SER:O     | 10:AK:58:THR:C     | 2.59                     | 0.45              |
| 20:AB:26:MET:HG2   | 20:AB:192:PRO:HG3  | 1.98                     | 0.45              |
| 21:AU:32:ARG:HB3   | 21:AU:33:ARG:H     | 1.59                     | 0.45              |
| 23:BB:359:G:C2'    | 23:BB:360:U:H5'    | 2.46                     | 0.45              |
| 23:BB:532:A:H2'    | 23:BB:532:A:N3     | 2.30                     | 0.45              |
| 23:BB:570:G:O2'    | 23:BB:571:U:H5'    | 2.16                     | 0.45              |
| 23:BB:630:G:H4'    | 23:BB:640:C:O2'    | 2.16                     | 0.45              |
| 23:BB:917:A:H2'    | 23:BB:918:A:O4'    | 2.15                     | 0.45              |
| 23:BB:963:U:H2'    | 23:BB:964:C:C6     | 2.51                     | 0.45              |
| 23:BB:1064:C:O2'   | 23:BB:1065:U:H5'   | 2.16                     | 0.45              |
| 23:BB:1123:C:H2'   | 23:BB:1124:G:C8    | 2.48                     | 0.45              |
| 23:BB:1157:G:H1'   | 45:BY:10:ARG:HH22  | 1.81                     | 0.45              |
| 23:BB:1940:U:H1'   | 23:BB:1941:C:H5    | 1.81                     | 0.45              |
| 23:BB:2721:A:H2'   | 23:BB:2722:G:C8    | 2.51                     | 0.45              |
| 23:BB:2748:A:H1'   | 29:BG:66:THR:OG1   | 2.16                     | 0.45              |
| 26:BD:50:VAL:HB    | 26:BD:75:ALA:HB3   | 1.97                     | 0.45              |
| 28:BF:32:LYS:HB3   | 28:BF:91:ARG:HB3   | 1.98                     | 0.45              |
| 29:BG:57:TYR:CZ    | 29:BG:59:ASP:HB2   | 2.52                     | 0.45              |
| 29:BG:71:LEU:HG    | 29:BG:74:MET:SD    | 2.56                     | 0.45              |
| 29:BG:169:ARG:C    | 29:BG:171:LYS:N    | 2.72                     | 0.45              |
| 31:BJ:19:ASP:O     | 31:BJ:20:ALA:HB3   | 2.16                     | 0.45              |
| 31:BJ:35:ARG:C     | 31:BJ:37:ARG:H     | 2.24                     | 0.45              |
| 33:BL:77:ILE:HB    | 33:BL:110:VAL:HG13 | 1.98                     | 0.45              |
| 33:BL:125:LEU:O    | 33:BL:126:ARG:HG3  | 2.17                     | 0.45              |
| 34:BM:124:LEU:HD23 | 34:BM:124:LEU:H    | 1.81                     | 0.45              |
| 37:BP:88:ARG:HA    | 37:BP:88:ARG:NE    | 2.30                     | 0.45              |
| 38:BQ:21:LYS:C     | 38:BQ:23:TYR:H     | 2.23                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 39:BR:42:ALA:O   | 39:BR:45:GLU:HG3   | 2.16                     | 0.45              |
| 40:BS:8:ARG:NH2  | 40:BS:102:HIS:NE2  | 2.64                     | 0.45              |
| 46:BZ:63:ARG:HA  | 46:BZ:63:ARG:NE    | 2.31                     | 0.45              |
| 48:B1:12:SER:HA  | 48:B1:50:GLU:CB    | 2.41                     | 0.45              |
| 50:B3:35:LYS:HD3 | 50:B3:35:LYS:N     | 2.31                     | 0.45              |
| 1:CA:202:G:N2    | 1:CA:465:A:H61     | 2.14                     | 0.45              |
| 1:CA:357:G:OP1   | 1:CA:367:U:H6      | 1.99                     | 0.45              |
| 1:CA:598:U:H2'   | 1:CA:599:C:C6      | 2.51                     | 0.45              |
| 1:CA:767:A:H2'   | 1:CA:768:A:H8      | 1.81                     | 0.45              |
| 1:CA:834:U:H2'   | 1:CA:835:U:C6      | 2.50                     | 0.45              |
| 1:CA:924:C:H2'   | 1:CA:925:G:H8      | 1.82                     | 0.45              |
| 1:CA:1014:A:H5'' | 18:CS:13:HIS:CB    | 2.46                     | 0.45              |
| 1:CA:1226:C:N4   | 12:CM:102:LYS:HZ3  | 2.14                     | 0.45              |
| 1:CA:1237:C:H3'  | 1:CA:1336:C:H41    | 1.81                     | 0.45              |
| 1:CA:1250:A:H5'' | 8:CI:69:GLY:H      | 1.81                     | 0.45              |
| 2:CC:145:ALA:HA  | 2:CC:203:LYS:HA    | 1.98                     | 0.45              |
| 3:CD:127:ARG:H   | 3:CD:127:ARG:CD    | 2.28                     | 0.45              |
| 4:CE:14:LEU:C    | 4:CE:14:LEU:HD13   | 2.41                     | 0.45              |
| 5:CF:67:PRO:O    | 5:CF:70:VAL:HG22   | 2.15                     | 0.45              |
| 8:CI:94:ARG:O    | 8:CI:98:ARG:HG3    | 2.15                     | 0.45              |
| 14:CO:36:ASN:HA  | 14:CO:39:GLN:HG3   | 1.98                     | 0.45              |
| 16:CQ:56:ASP:N   | 16:CQ:81:ALA:HB2   | 2.31                     | 0.45              |
| 18:CS:24:SER:HB2 | 18:CS:27:LYS:HZ1   | 1.79                     | 0.45              |
| 20:CB:67:LEU:O   | 20:CB:160:LEU:HD12 | 2.16                     | 0.45              |
| 23:DB:299:A:N6   | 23:DB:322:A:H1'    | 2.31                     | 0.45              |
| 23:DB:346:A:H2'  | 23:DB:347:A:O4'    | 2.15                     | 0.45              |
| 23:DB:383:C:H41  | 23:DB:385:C:H2'    | 1.81                     | 0.45              |
| 23:DB:448:U:C6   | 27:DE:79:ARG:HG3   | 2.51                     | 0.45              |
| 23:DB:786:C:H5'' | 23:DB:1780:A:N7    | 2.31                     | 0.45              |
| 23:DB:873:C:H4'  | 34:DM:64:TRP:CZ3   | 2.51                     | 0.45              |
| 23:DB:1033:U:C4  | 51:D4:16:ILE:HD11  | 2.52                     | 0.45              |
| 23:DB:1084:A:H1' | 23:DB:1106:G:H5'   | 1.98                     | 0.45              |
| 23:DB:1678:A:O2' | 23:DB:1679:A:H5'   | 2.16                     | 0.45              |
| 23:DB:1747:U:H2' | 23:DB:1748:C:H6    | 1.80                     | 0.45              |
| 23:DB:1816:C:C5  | 25:DC:62:ARG:HD2   | 2.51                     | 0.45              |
| 23:DB:1821:A:C5' | 25:DC:155:ARG:HH21 | 2.29                     | 0.45              |
| 23:DB:2087:G:H2' | 23:DB:2088:A:C8    | 2.51                     | 0.45              |
| 23:DB:2182:U:H2' | 23:DB:2183:A:C8    | 2.52                     | 0.45              |
| 23:DB:2379:G:H2' | 23:DB:2380:C:C6    | 2.51                     | 0.45              |
| 23:DB:2477:U:H4' | 23:DB:2479:U:O4    | 2.16                     | 0.45              |
| 23:DB:2746:U:O2' | 23:DB:2747:G:H5'   | 2.16                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:DC:142:ASN:HA   | 25:DC:153:LEU:CD2 | 2.46                     | 0.45              |
| 26:DD:138:LEU:HD12 | 26:DD:142:VAL:HB  | 1.98                     | 0.45              |
| 27:DE:55:SER:N     | 27:DE:74:LYS:HE3  | 2.30                     | 0.45              |
| 32:DK:12:ASP:HA    | 32:DK:99:ILE:HA   | 1.97                     | 0.45              |
| 33:DL:18:ARG:NH2   | 33:DL:21:ARG:HD3  | 2.31                     | 0.45              |
| 34:DM:85:GLY:O     | 34:DM:86:LYS:O    | 2.34                     | 0.45              |
| 35:DN:103:ARG:O    | 35:DN:104:ALA:HB3 | 2.15                     | 0.45              |
| 37:DP:52:ARG:HG3   | 37:DP:54:LEU:HD12 | 1.98                     | 0.45              |
| 41:DT:20:ALA:O     | 41:DT:21:SER:HB3  | 2.17                     | 0.45              |
| 45:DY:37:ARG:HA    | 45:DY:37:ARG:NE   | 2.31                     | 0.45              |
| 49:D2:46:LYS:HE3   | 49:D2:46:LYS:N    | 2.31                     | 0.45              |
| 1:AA:22:G:O2'      | 1:AA:23:C:H5'     | 2.17                     | 0.45              |
| 1:AA:336:A:O2'     | 1:AA:337:G:H5'    | 2.15                     | 0.45              |
| 1:AA:411:A:C5      | 1:AA:413:G:H1'    | 2.51                     | 0.45              |
| 1:AA:767:A:H2'     | 1:AA:768:A:H8     | 1.81                     | 0.45              |
| 1:AA:880:C:H2'     | 1:AA:881:G:H8     | 1.81                     | 0.45              |
| 1:AA:1430:A:H2'    | 1:AA:1431:A:O4'   | 2.17                     | 0.45              |
| 1:AA:1473:G:H2'    | 1:AA:1474:U:O4'   | 2.16                     | 0.45              |
| 2:AC:70:ALA:HB2    | 2:AC:108:PRO:HB3  | 1.99                     | 0.45              |
| 3:AD:56:GLU:HG2    | 3:AD:198:LEU:HD12 | 1.97                     | 0.45              |
| 3:AD:64:TYR:H      | 3:AD:64:TYR:HD1   | 1.64                     | 0.45              |
| 5:AF:7:VAL:O       | 5:AF:7:VAL:HG13   | 2.16                     | 0.45              |
| 6:AG:11:ILE:H      | 6:AG:11:ILE:HD12  | 1.80                     | 0.45              |
| 7:AH:75:GLN:O      | 7:AH:126:CYS:HB2  | 2.17                     | 0.45              |
| 7:AH:104:SER:O     | 7:AH:122:GLY:HA3  | 2.16                     | 0.45              |
| 10:AK:22:ILE:HD12  | 10:AK:85:VAL:HG22 | 1.98                     | 0.45              |
| 11:AL:31:GLY:HA3   | 11:AL:54:VAL:CG1  | 2.46                     | 0.45              |
| 15:AP:45:GLU:HG2   | 15:AP:45:GLU:O    | 2.16                     | 0.45              |
| 18:AS:11:ASP:HB2   | 18:AS:14:LEU:CD2  | 2.47                     | 0.45              |
| 23:BB:125:A:H5'    | 49:B2:19:ARG:HE   | 1.81                     | 0.45              |
| 23:BB:528:A:N1     | 23:BB:2043:C:H5'  | 2.31                     | 0.45              |
| 23:BB:764:A:N1     | 23:BB:1789:A:O2'  | 2.47                     | 0.45              |
| 23:BB:1047:G:HO2'  | 23:BB:1048:A:P    | 2.39                     | 0.45              |
| 23:BB:1112:G:O2'   | 29:BG:2:ARG:HG2   | 2.17                     | 0.45              |
| 23:BB:1133:A:H4'   | 23:BB:1134:A:C5'  | 2.46                     | 0.45              |
| 23:BB:1164:C:H2'   | 23:BB:1165:A:H8   | 1.81                     | 0.45              |
| 23:BB:1184:U:H2'   | 23:BB:1185:G:H8   | 1.81                     | 0.45              |
| 23:BB:1541:C:H2'   | 23:BB:1542:U:O4'  | 2.16                     | 0.45              |
| 23:BB:1597:A:H5''  | 23:BB:1598:A:H5'  | 1.97                     | 0.45              |
| 23:BB:1760:C:H2'   | 23:BB:1761:C:O4'  | 2.16                     | 0.45              |
| 23:BB:1790:C:H2'   | 23:BB:1791:A:C8   | 2.51                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:1803:A:H2    | 23:BB:1823:G:C1'   | 2.29                     | 0.45              |
| 23:BB:1915:U:H3'   | 23:BB:1916:A:C8    | 2.50                     | 0.45              |
| 23:BB:2056:G:O2'   | 47:B0:2:VAL:HG11   | 2.17                     | 0.45              |
| 23:BB:2276:G:OP2   | 34:BM:83:GLY:HA3   | 2.16                     | 0.45              |
| 25:BC:38:LYS:O     | 25:BC:39:SER:HB3   | 2.15                     | 0.45              |
| 26:BD:128:ARG:NH2  | 26:BD:130:GLN:CD   | 2.74                     | 0.45              |
| 26:BD:146:ILE:HG21 | 26:BD:159:LYS:NZ   | 2.30                     | 0.45              |
| 26:BD:184:ARG:O    | 26:BD:184:ARG:HG3  | 2.16                     | 0.45              |
| 29:BG:104:LEU:HD12 | 29:BG:104:LEU:N    | 2.31                     | 0.45              |
| 31:BJ:31:GLU:O     | 31:BJ:35:ARG:HB2   | 2.15                     | 0.45              |
| 33:BL:77:ILE:HG22  | 33:BL:78:ARG:N     | 2.30                     | 0.45              |
| 42:BU:3:LYS:HD2    | 42:BU:81:ARG:HH22  | 1.81                     | 0.45              |
| 49:B2:38:GLY:O     | 49:B2:39:ARG:C     | 2.58                     | 0.45              |
| 52:BI:121:ILE:O    | 52:BI:124:MET:HG2  | 2.16                     | 0.45              |
| 1:CA:720:C:O4'     | 17:CR:38:ILE:HG12  | 2.16                     | 0.45              |
| 1:CA:744:C:H2'     | 1:CA:745:G:C8      | 2.50                     | 0.45              |
| 2:CC:38:VAL:O      | 2:CC:42:LEU:HD23   | 2.17                     | 0.45              |
| 2:CC:76:ILE:HA     | 2:CC:83:VAL:CG2    | 2.46                     | 0.45              |
| 2:CC:94:ALA:O      | 2:CC:96:VAL:N      | 2.50                     | 0.45              |
| 3:CD:47:LEU:HD11   | 3:CD:52:VAL:N      | 2.31                     | 0.45              |
| 3:CD:54:LEU:O      | 3:CD:58:GLN:HB2    | 2.17                     | 0.45              |
| 3:CD:160:LEU:HD13  | 3:CD:160:LEU:C     | 2.41                     | 0.45              |
| 4:CE:156:ARG:NH2   | 7:CH:100:ILE:HG23  | 2.32                     | 0.45              |
| 6:CG:41:ILE:HD13   | 6:CG:115:MET:HG3   | 1.97                     | 0.45              |
| 7:CH:45:ILE:CD1    | 7:CH:60:LEU:HD11   | 2.46                     | 0.45              |
| 9:CJ:8:ILE:HD11    | 9:CJ:74:VAL:HB     | 1.98                     | 0.45              |
| 9:CJ:17:LEU:HD22   | 9:CJ:17:LEU:O      | 2.16                     | 0.45              |
| 14:CO:10:ILE:HG21  | 14:CO:30:LEU:CD2   | 2.45                     | 0.45              |
| 16:CQ:10:ARG:CZ    | 16:CQ:55:GLY:N     | 2.79                     | 0.45              |
| 20:CB:95:TRP:CZ2   | 20:CB:100:LEU:HD13 | 2.50                     | 0.45              |
| 22:DA:55:U:H2'     | 22:DA:56:G:C8      | 2.51                     | 0.45              |
| 23:DB:257:C:H2'    | 23:DB:258:G:O4'    | 2.17                     | 0.45              |
| 23:DB:264:C:H2'    | 23:DB:265:A:H5''   | 1.98                     | 0.45              |
| 23:DB:315:G:O2'    | 23:DB:316:C:H5'    | 2.16                     | 0.45              |
| 23:DB:439:A:H2'    | 23:DB:440:C:O4'    | 2.16                     | 0.45              |
| 23:DB:630:G:H4'    | 23:DB:640:C:O2'    | 2.16                     | 0.45              |
| 23:DB:692:C:H2'    | 23:DB:693:A:H8     | 1.80                     | 0.45              |
| 23:DB:1353:A:H2'   | 23:DB:1354:A:C8    | 2.50                     | 0.45              |
| 23:DB:1683:U:H2'   | 23:DB:1684:G:C8    | 2.51                     | 0.45              |
| 23:DB:1704:C:O2'   | 23:DB:1705:A:H5'   | 2.16                     | 0.45              |
| 23:DB:1910:G:O2'   | 23:DB:1911:U:H5'   | 2.16                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:1979:U:C2'  | 23:DB:1980:G:H5'   | 2.45                     | 0.45              |
| 23:DB:2038:G:H2'  | 23:DB:2039:U:O4'   | 2.17                     | 0.45              |
| 25:DC:171:VAL:O   | 25:DC:172:THR:HG23 | 2.17                     | 0.45              |
| 25:DC:235:GLU:CG  | 25:DC:237:ARG:HD3  | 2.46                     | 0.45              |
| 30:DH:109:GLU:O   | 30:DH:109:GLU:HG3  | 2.16                     | 0.45              |
| 30:DH:126:GLY:H   | 30:DH:146:VAL:HB   | 1.82                     | 0.45              |
| 31:DJ:90:GLU:C    | 31:DJ:92:MET:N     | 2.73                     | 0.45              |
| 32:DK:78:ARG:H    | 37:DP:72:VAL:CG2   | 2.27                     | 0.45              |
| 32:DK:87:LEU:HD22 | 32:DK:92:GLU:O     | 2.17                     | 0.45              |
| 33:DL:77:ILE:HD13 | 33:DL:110:VAL:CA   | 2.44                     | 0.45              |
| 34:DM:127:LYS:HD3 | 34:DM:127:LYS:C    | 2.41                     | 0.45              |
| 35:DN:48:VAL:O    | 35:DN:51:LEU:HB2   | 2.15                     | 0.45              |
| 36:DO:27:VAL:HG22 | 36:DO:38:GLN:O     | 2.17                     | 0.45              |
| 36:DO:30:ARG:CG   | 36:DO:31:THR:H     | 2.28                     | 0.45              |
| 38:DQ:88:GLU:OE2  | 39:DR:53:PHE:HB2   | 2.16                     | 0.45              |
| 39:DR:4:VAL:O     | 39:DR:41:ILE:HG21  | 2.16                     | 0.45              |
| 40:DS:87:PRO:O    | 40:DS:88:ARG:CB    | 2.64                     | 0.45              |
| 41:DT:38:ALA:HB1  | 41:DT:43:ILE:CD1   | 2.42                     | 0.45              |
| 44:DX:7:ARG:C     | 44:DX:8:GLU:HG3    | 2.41                     | 0.45              |
| 46:DZ:37:CYS:SG   | 46:DZ:39:LYS:HB2   | 2.57                     | 0.45              |
| 1:AA:167:A:H2'    | 1:AA:168:G:H8      | 1.81                     | 0.45              |
| 1:AA:299:G:H2'    | 1:AA:300:A:C8      | 2.51                     | 0.45              |
| 1:AA:1206:G:H4'   | 2:AC:192:TYR:HA    | 1.98                     | 0.45              |
| 1:AA:1490:U:H5'   | 1:AA:1491:G:OP2    | 2.16                     | 0.45              |
| 12:AM:47:LEU:HB3  | 12:AM:51:GLN:HB2   | 1.97                     | 0.45              |
| 12:AM:102:LYS:HB2 | 12:AM:102:LYS:NZ   | 2.31                     | 0.45              |
| 17:AR:62:ARG:HD3  | 17:AR:69:TYR:HA    | 1.99                     | 0.45              |
| 18:AS:43:MET:O    | 18:AS:46:LEU:HB2   | 2.16                     | 0.45              |
| 23:BB:28:A:H1'    | 23:BB:513:A:C2     | 2.52                     | 0.45              |
| 23:BB:492:A:H2'   | 23:BB:493:G:O4'    | 2.16                     | 0.45              |
| 23:BB:997:G:C5'   | 38:BQ:91:ARG:HG3   | 2.47                     | 0.45              |
| 23:BB:1289:C:H2'  | 23:BB:1290:C:C6    | 2.51                     | 0.45              |
| 23:BB:1720:U:C2'  | 23:BB:1721:G:H5'   | 2.46                     | 0.45              |
| 23:BB:1818:U:H2'  | 25:BC:152:GLN:O    | 2.17                     | 0.45              |
| 23:BB:2261:C:O2'  | 23:BB:2262:U:H5'   | 2.15                     | 0.45              |
| 23:BB:2512:C:O2'  | 26:BD:146:ILE:HG12 | 2.15                     | 0.45              |
| 23:BB:2800:A:C4   | 23:BB:2801:G:H1'   | 2.51                     | 0.45              |
| 24:BV:44:HIS:O    | 24:BV:48:MET:HB3   | 2.16                     | 0.45              |
| 25:BC:68:ARG:HD2  | 25:BC:127:ASN:ND2  | 2.27                     | 0.45              |
| 25:BC:140:VAL:HA  | 25:BC:191:LEU:HA   | 1.98                     | 0.45              |
| 27:BE:6:LYS:HB2   | 27:BE:12:LEU:CD1   | 2.46                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BE:146:VAL:HG23 | 27:BE:148:ILE:CG2  | 2.46                     | 0.45              |
| 28:BF:15:LEU:HD13  | 28:BF:28:PRO:CG    | 2.45                     | 0.45              |
| 28:BF:33:ILE:HG22  | 28:BF:155:ILE:HA   | 1.98                     | 0.45              |
| 30:BH:41:LYS:O     | 30:BH:42:LYS:C     | 2.59                     | 0.45              |
| 31:BJ:25:LEU:HD13  | 31:BJ:25:LEU:H     | 1.81                     | 0.45              |
| 31:BJ:25:LEU:CD1   | 31:BJ:62:VAL:HA    | 2.41                     | 0.45              |
| 31:BJ:50:THR:OG1   | 31:BJ:51:GLY:N     | 2.49                     | 0.45              |
| 34:BM:8:LYS:NZ     | 34:BM:70:ASP:H     | 2.10                     | 0.45              |
| 35:BN:9:GLN:NE2    | 35:BN:17:ARG:NH2   | 2.65                     | 0.45              |
| 35:BN:86:ARG:NH2   | 35:BN:116:VAL:HG11 | 2.31                     | 0.45              |
| 36:BO:31:THR:HG21  | 36:BO:36:TYR:HE1   | 1.82                     | 0.45              |
| 37:BP:60:VAL:HB    | 37:BP:61:ARG:H     | 1.46                     | 0.45              |
| 40:BS:69:LEU:HA    | 40:BS:108:SER:O    | 2.16                     | 0.45              |
| 41:BT:57:VAL:O     | 41:BT:85:VAL:HA    | 2.16                     | 0.45              |
| 43:BW:58:LEU:HA    | 43:BW:79:ILE:HG22  | 1.98                     | 0.45              |
| 45:BY:29:ARG:O     | 45:BY:30:ARG:HB2   | 2.17                     | 0.45              |
| 50:B3:12:ARG:HB2   | 50:B3:12:ARG:CZ    | 2.41                     | 0.45              |
| 50:B3:16:THR:HG21  | 50:B3:22:LYS:NZ    | 2.32                     | 0.45              |
| 51:B4:7:VAL:HG12   | 51:B4:8:LYS:N      | 2.25                     | 0.45              |
| 1:CA:7:A:H2        | 4:CE:125:LYS:HE2   | 1.82                     | 0.45              |
| 1:CA:167:A:H2'     | 1:CA:168:G:H8      | 1.81                     | 0.45              |
| 1:CA:299:G:H2'     | 1:CA:300:A:C8      | 2.51                     | 0.45              |
| 1:CA:393:A:H5'     | 1:CA:483:C:O2'     | 2.15                     | 0.45              |
| 1:CA:977:A:H8      | 1:CA:1223:C:N3     | 2.15                     | 0.45              |
| 1:CA:1000:A:O2'    | 1:CA:1001:C:H5'    | 2.16                     | 0.45              |
| 1:CA:1004:A:N7     | 1:CA:1025:U:O2'    | 2.48                     | 0.45              |
| 1:CA:1013:G:N2     | 1:CA:1015:G:H3'    | 2.32                     | 0.45              |
| 1:CA:1054:C:O2'    | 1:CA:1055:A:H5''   | 2.17                     | 0.45              |
| 1:CA:1124:G:H5'    | 9:CJ:37:ARG:HH21   | 1.81                     | 0.45              |
| 1:CA:1187:G:H2'    | 1:CA:1188:A:O4'    | 2.16                     | 0.45              |
| 1:CA:1308:U:OP2    | 12:CM:97:ARG:HD3   | 2.16                     | 0.45              |
| 1:CA:1456:A:H2'    | 1:CA:1457:G:H8     | 1.81                     | 0.45              |
| 2:CC:99:GLN:O      | 2:CC:100:ILE:HB    | 2.16                     | 0.45              |
| 3:CD:30:LYS:HD3    | 3:CD:30:LYS:N      | 2.31                     | 0.45              |
| 8:CI:56:MET:HA     | 8:CI:59:LYS:HB2    | 1.98                     | 0.45              |
| 9:CJ:36:VAL:HG22   | 9:CJ:76:ILE:HD13   | 1.98                     | 0.45              |
| 10:CK:126:ARG:HH11 | 10:CK:126:ARG:HG2  | 1.80                     | 0.45              |
| 12:CM:48:SER:C     | 12:CM:50:GLY:H     | 2.23                     | 0.45              |
| 12:CM:79:LEU:HB2   | 12:CM:84:CYS:SG    | 2.57                     | 0.45              |
| 16:CQ:74:LEU:HD22  | 16:CQ:75:VAL:H     | 1.82                     | 0.45              |
| 17:CR:61:ALA:HB3   | 17:CR:67:LEU:HD12  | 1.98                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 19:CT:19:HIS:CE1   | 19:CT:23:ARG:HG3  | 2.51                     | 0.45              |
| 20:CB:60:ALA:HB2   | 20:CB:66:ILE:HD11 | 1.98                     | 0.45              |
| 20:CB:148:GLY:C    | 20:CB:150:ILE:H   | 2.24                     | 0.45              |
| 20:CB:209:VAL:HG23 | 20:CB:210:THR:N   | 2.31                     | 0.45              |
| 22:DA:12:C:H4'     | 22:DA:15:A:N6     | 2.32                     | 0.45              |
| 22:DA:63:C:H2'     | 22:DA:64:G:C8     | 2.51                     | 0.45              |
| 23:DB:137:U:O2'    | 23:DB:138:U:H5'   | 2.16                     | 0.45              |
| 23:DB:265:A:O2'    | 23:DB:266:G:H4'   | 2.17                     | 0.45              |
| 23:DB:345:A:N3     | 23:DB:346:A:N1    | 2.64                     | 0.45              |
| 23:DB:522:A:H2'    | 23:DB:523:C:H6    | 1.80                     | 0.45              |
| 23:DB:709:U:H2'    | 23:DB:710:U:C6    | 2.51                     | 0.45              |
| 23:DB:780:G:OP1    | 25:DC:216:ARG:NH2 | 2.49                     | 0.45              |
| 23:DB:1047:G:H1'   | 23:DB:1110:G:N2   | 2.32                     | 0.45              |
| 23:DB:1099:G:C4'   | 52:DI:4:VAL:HB    | 2.43                     | 0.45              |
| 23:DB:1289:C:H2'   | 23:DB:1290:C:C6   | 2.51                     | 0.45              |
| 23:DB:1313:U:O2    | 23:DB:1313:U:C2'  | 2.64                     | 0.45              |
| 23:DB:1322:A:H2'   | 23:DB:1323:C:H5'  | 1.98                     | 0.45              |
| 23:DB:1601:G:O2'   | 23:DB:1602:U:H5'  | 2.16                     | 0.45              |
| 23:DB:1668:A:N3    | 23:DB:1670:C:C4   | 2.84                     | 0.45              |
| 23:DB:1708:C:H2'   | 23:DB:1709:U:H6   | 1.82                     | 0.45              |
| 23:DB:2103:C:H3'   | 23:DB:2104:C:C2   | 2.51                     | 0.45              |
| 23:DB:2147:A:N3    | 23:DB:2147:A:C2'  | 2.78                     | 0.45              |
| 23:DB:2207:C:H2'   | 23:DB:2208:C:H6   | 1.82                     | 0.45              |
| 23:DB:2465:C:O2'   | 23:DB:2466:C:H5'  | 2.17                     | 0.45              |
| 23:DB:2772:C:H2'   | 23:DB:2773:C:H6   | 1.81                     | 0.45              |
| 23:DB:2830:C:O2'   | 23:DB:2831:G:H5'  | 2.17                     | 0.45              |
| 24:DV:65:VAL:O     | 24:DV:66:ASP:HB3  | 2.15                     | 0.45              |
| 24:DV:93:ARG:HG2   | 24:DV:94:ALA:H    | 1.82                     | 0.45              |
| 25:DC:19:VAL:CG1   | 25:DC:20:ASN:N    | 2.80                     | 0.45              |
| 26:DD:100:LEU:HD13 | 26:DD:100:LEU:C   | 2.41                     | 0.45              |
| 27:DE:4:VAL:HA     | 27:DE:14:VAL:CG1  | 2.46                     | 0.45              |
| 28:DF:70:ARG:HA    | 28:DF:80:GLN:NE2  | 2.20                     | 0.45              |
| 28:DF:108:PRO:O    | 28:DF:109:ARG:HB2 | 2.17                     | 0.45              |
| 29:DG:131:VAL:HG13 | 29:DG:131:VAL:O   | 2.15                     | 0.45              |
| 29:DG:171:LYS:HB2  | 29:DG:172:GLU:H   | 1.61                     | 0.45              |
| 30:DH:92:GLY:O     | 30:DH:93:SER:HB3  | 2.16                     | 0.45              |
| 35:DN:16:HIS:O     | 35:DN:20:MET:N    | 2.41                     | 0.45              |
| 36:DO:25:ARG:HG2   | 36:DO:94:ARG:NH2  | 2.27                     | 0.45              |
| 38:DQ:52:ARG:HG2   | 38:DQ:53:LYS:CE   | 2.46                     | 0.45              |
| 40:DS:46:LEU:CA    | 40:DS:49:LYS:HB2  | 2.32                     | 0.45              |
| 40:DS:85:ILE:HG12  | 40:DS:94:ASP:O    | 2.16                     | 0.45              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 41:DT:30:ILE:O    | 41:DT:85:VAL:HG22  | 2.17                     | 0.45              |
| 45:DY:6:ILE:HG13  | 45:DY:6:ILE:O      | 2.16                     | 0.45              |
| 45:DY:24:LEU:C    | 45:DY:26:LEU:N     | 2.74                     | 0.45              |
| 46:DZ:1:MET:C     | 46:DZ:2:LYS:HG3    | 2.41                     | 0.45              |
| 46:DZ:25:ARG:CG   | 46:DZ:26:SER:H     | 2.22                     | 0.45              |
| 52:DI:9:LYS:HG2   | 52:DI:57:VAL:HG13  | 1.98                     | 0.45              |
| 52:DI:96:LYS:HD3  | 52:DI:138:VAL:HG21 | 1.96                     | 0.45              |
| 1:AA:708:C:H2'    | 1:AA:709:U:H6      | 1.79                     | 0.45              |
| 1:AA:744:C:H2'    | 1:AA:745:G:C8      | 2.50                     | 0.45              |
| 1:AA:836:G:H2'    | 1:AA:837:U:C6      | 2.52                     | 0.45              |
| 1:AA:962:C:H2'    | 1:AA:963:G:O4'     | 2.17                     | 0.45              |
| 1:AA:1258:G:C4    | 1:AA:1278:G:N2     | 2.84                     | 0.45              |
| 2:AC:40:GLN:CD    | 2:AC:44:LYS:HD2    | 2.42                     | 0.45              |
| 2:AC:141:MET:HE2  | 2:AC:145:ALA:O     | 2.16                     | 0.45              |
| 2:AC:186:SER:O    | 2:AC:197:VAL:HG12  | 2.16                     | 0.45              |
| 3:AD:163:GLN:N    | 3:AD:163:GLN:OE1   | 2.50                     | 0.45              |
| 4:AE:81:GLN:NE2   | 4:AE:147:ASN:N     | 2.65                     | 0.45              |
| 7:AH:47:ASP:CG    | 7:AH:48:PHE:H      | 2.25                     | 0.45              |
| 7:AH:48:PHE:HB2   | 7:AH:60:LEU:HD12   | 1.99                     | 0.45              |
| 7:AH:113:ARG:C    | 7:AH:113:ARG:HE    | 2.23                     | 0.45              |
| 8:AI:33:SER:C     | 8:AI:35:GLU:N      | 2.74                     | 0.45              |
| 10:AK:112:VAL:HA  | 17:AR:72:ARG:HD3   | 1.99                     | 0.45              |
| 14:AO:78:THR:HA   | 14:AO:81:ILE:CD1   | 2.46                     | 0.45              |
| 15:AP:29:ASN:N    | 15:AP:29:ASN:ND2   | 2.63                     | 0.45              |
| 15:AP:71:VAL:HA   | 15:AP:74:LEU:CG    | 2.45                     | 0.45              |
| 20:AB:72:LYS:NZ   | 20:AB:167:HIS:HB2  | 2.32                     | 0.45              |
| 20:AB:96:LEU:HD21 | 20:AB:146:SER:HB2  | 1.98                     | 0.45              |
| 21:AU:43:GLU:HA   | 21:AU:43:GLU:OE1   | 2.15                     | 0.45              |
| 22:BA:29:A:H3'    | 22:BA:30:C:C6      | 2.49                     | 0.45              |
| 22:BA:64:G:O2'    | 22:BA:65:U:H5'     | 2.17                     | 0.45              |
| 23:BB:6:A:H5''    | 31:BJ:133:ALA:O    | 2.17                     | 0.45              |
| 23:BB:48:G:H4'    | 23:BB:52:A:O4'     | 2.16                     | 0.45              |
| 23:BB:189:G:H2'   | 23:BB:205:G:H22    | 1.81                     | 0.45              |
| 23:BB:327:G:O2'   | 23:BB:328:U:H5'    | 2.16                     | 0.45              |
| 23:BB:407:G:O2'   | 23:BB:408:G:H5'    | 2.16                     | 0.45              |
| 23:BB:760:G:H4'   | 23:BB:1776:G:OP1   | 2.16                     | 0.45              |
| 23:BB:1060:U:C4   | 52:BI:131:THR:HG22 | 2.51                     | 0.45              |
| 23:BB:1665:A:O2'  | 23:BB:1666:G:H5'   | 2.15                     | 0.45              |
| 23:BB:2038:G:H2'  | 23:BB:2039:U:O4'   | 2.17                     | 0.45              |
| 23:BB:2038:G:H2'  | 23:BB:2039:U:H6    | 1.82                     | 0.45              |
| 23:BB:2301:C:O2'  | 23:BB:2302:U:H5'   | 2.17                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:2363:G:O2'  | 23:BB:2364:C:H5'   | 2.17                     | 0.45              |
| 23:BB:2556:C:O2'  | 23:BB:2557:G:H5'   | 2.17                     | 0.45              |
| 25:BC:136:VAL:HA  | 25:BC:165:ALA:HA   | 1.99                     | 0.45              |
| 26:BD:12:THR:HB   | 26:BD:21:SER:O     | 2.15                     | 0.45              |
| 26:BD:115:GLY:HA2 | 26:BD:165:MET:CG   | 2.35                     | 0.45              |
| 27:BE:194:LYS:HE3 | 27:BE:201:ALA:HB2  | 1.98                     | 0.45              |
| 29:BG:25:ILE:HD11 | 29:BG:75:VAL:HG12  | 1.97                     | 0.45              |
| 29:BG:51:PHE:H    | 29:BG:68:ARG:HD3   | 1.80                     | 0.45              |
| 31:BJ:120:ARG:O   | 31:BJ:122:LEU:N    | 2.42                     | 0.45              |
| 33:BL:82:LEU:HG   | 33:BL:122:VAL:HG12 | 1.99                     | 0.45              |
| 33:BL:84:LYS:C    | 33:BL:86:GLU:H     | 2.25                     | 0.45              |
| 34:BM:70:ASP:C    | 34:BM:71:LYS:HG3   | 2.41                     | 0.45              |
| 36:BO:97:PHE:O    | 36:BO:98:GLN:HG2   | 2.16                     | 0.45              |
| 38:BQ:12:ARG:HH11 | 38:BQ:12:ARG:HG2   | 1.82                     | 0.45              |
| 39:BR:14:VAL:HG12 | 39:BR:15:SER:N     | 2.32                     | 0.45              |
| 39:BR:53:PHE:HD2  | 39:BR:55:ASP:H     | 1.59                     | 0.45              |
| 40:BS:88:ARG:HB3  | 40:BS:89:ALA:H     | 1.57                     | 0.45              |
| 40:BS:102:HIS:O   | 40:BS:103:ILE:HB   | 2.15                     | 0.45              |
| 46:BZ:19:GLY:O    | 46:BZ:20:ASN:HB2   | 2.16                     | 0.45              |
| 47:B0:54:ILE:O    | 47:B0:54:ILE:HG13  | 2.17                     | 0.45              |
| 48:B1:41:VAL:HB   | 48:B1:43:ARG:NH2   | 2.31                     | 0.45              |
| 50:B3:26:ALA:HB3  | 50:B3:29:ARG:CZ    | 2.46                     | 0.45              |
| 1:CA:29:U:H5'     | 1:CA:296:U:OP1     | 2.17                     | 0.45              |
| 1:CA:328:C:H4'    | 1:CA:329:A:H5''    | 1.98                     | 0.45              |
| 1:CA:525:C:H2'    | 1:CA:526:C:C6      | 2.51                     | 0.45              |
| 1:CA:812:G:N3     | 1:CA:812:G:C2'     | 2.77                     | 0.45              |
| 1:CA:1108:G:H5''  | 2:CC:175:HIS:HD1   | 1.82                     | 0.45              |
| 1:CA:1309:G:C5'   | 12:CM:76:ILE:HG12  | 2.46                     | 0.45              |
| 3:CD:141:VAL:HG12 | 3:CD:180:THR:CA    | 2.45                     | 0.45              |
| 5:CF:100:SER:N    | 17:CR:23:LYS:NZ    | 2.63                     | 0.45              |
| 8:CI:56:MET:C     | 8:CI:58:GLU:N      | 2.73                     | 0.45              |
| 10:CK:60:PHE:O    | 10:CK:64:VAL:HG13  | 2.15                     | 0.45              |
| 11:CL:36:VAL:HG12 | 11:CL:52:CYS:HB2   | 1.96                     | 0.45              |
| 15:CP:43:ALA:C    | 15:CP:45:GLU:H     | 2.23                     | 0.45              |
| 16:CQ:46:HIS:CG   | 16:CQ:47:ASP:H     | 2.33                     | 0.45              |
| 19:CT:34:VAL:CG1  | 19:CT:78:LEU:HD22  | 2.47                     | 0.45              |
| 20:CB:207:ARG:O   | 20:CB:208:ALA:C    | 2.59                     | 0.45              |
| 21:CU:23:GLU:HA   | 21:CU:27:VAL:HG21  | 1.98                     | 0.45              |
| 21:CU:39:LYS:N    | 21:CU:40:PRO:HD2   | 2.21                     | 0.45              |
| 23:DB:359:G:C2'   | 23:DB:360:U:H5'    | 2.46                     | 0.45              |
| 23:DB:534:U:H5'   | 38:DQ:41:ALA:CA    | 2.43                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DB:817:C:O2'    | 23:DB:839:U:H5''  | 2.17                     | 0.45              |
| 23:DB:1099:G:H5''  | 52:DI:2:LYS:HB2   | 1.98                     | 0.45              |
| 23:DB:1259:G:O2'   | 23:DB:1260:A:H5'  | 2.17                     | 0.45              |
| 23:DB:1408:G:H2'   | 23:DB:1409:U:H6   | 1.80                     | 0.45              |
| 23:DB:1553:A:O2'   | 23:DB:1554:U:H2'  | 2.16                     | 0.45              |
| 23:DB:2223:G:O2'   | 23:DB:2224:G:H5'  | 2.16                     | 0.45              |
| 23:DB:2243:U:O2    | 23:DB:2434:A:C2   | 2.69                     | 0.45              |
| 23:DB:2276:G:OP1   | 34:DM:82:MET:SD   | 2.75                     | 0.45              |
| 23:DB:2529:G:H4'   | 29:DG:175:LYS:HD3 | 1.98                     | 0.45              |
| 23:DB:2714:G:H2'   | 23:DB:2715:C:C6   | 2.51                     | 0.45              |
| 25:DC:152:GLN:HB3  | 25:DC:153:LEU:H   | 1.62                     | 0.45              |
| 25:DC:227:VAL:HG13 | 25:DC:228:ASP:OD1 | 2.17                     | 0.45              |
| 26:DD:33:ARG:C     | 26:DD:34:VAL:HG13 | 2.42                     | 0.45              |
| 27:DE:23:PHE:CG    | 27:DE:24:ASN:N    | 2.85                     | 0.45              |
| 27:DE:114:ARG:NH1  | 27:DE:114:ARG:HG3 | 2.32                     | 0.45              |
| 30:DH:4:ILE:HD11   | 30:DH:37:VAL:O    | 2.17                     | 0.45              |
| 31:DJ:85:LYS:NZ    | 31:DJ:86:GLN:O    | 2.49                     | 0.45              |
| 33:DL:50:PHE:O     | 33:DL:52:GLY:N    | 2.49                     | 0.45              |
| 33:DL:55:MET:SD    | 33:DL:56:PRO:HG3  | 2.56                     | 0.45              |
| 35:DN:52:ILE:HD11  | 35:DN:83:LEU:HD21 | 1.99                     | 0.45              |
| 35:DN:96:ARG:NH1   | 35:DN:98:LEU:HD21 | 2.31                     | 0.45              |
| 36:DO:30:ARG:O     | 36:DO:31:THR:HB   | 2.16                     | 0.45              |
| 39:DR:76:LYS:HB3   | 39:DR:90:ARG:HG2  | 1.96                     | 0.45              |
| 39:DR:99:THR:HG23  | 39:DR:100:GLY:H   | 1.80                     | 0.45              |
| 40:DS:81:SER:HB2   | 40:DS:99:ARG:H    | 1.81                     | 0.45              |
| 42:DU:95:PHE:HB2   | 42:DU:99:SER:C    | 2.41                     | 0.45              |
| 43:DW:36:ILE:HG21  | 43:DW:68:PHE:HE1  | 1.79                     | 0.45              |
| 1:AA:29:U:O2'      | 1:AA:30:U:H5'     | 2.17                     | 0.45              |
| 1:AA:718:A:H5'     | 10:AK:118:ASN:HB2 | 1.97                     | 0.45              |
| 1:AA:972:C:H4'     | 9:AJ:59:LYS:HB3   | 1.99                     | 0.45              |
| 1:AA:1014:A:OP2    | 18:AS:17:LYS:NZ   | 2.45                     | 0.45              |
| 1:AA:1113:C:H2'    | 1:AA:1114:C:H6    | 1.82                     | 0.45              |
| 1:AA:1197:A:P      | 1:AA:1197:A:H3'   | 2.57                     | 0.45              |
| 1:AA:1410:A:H2'    | 1:AA:1411:C:H6    | 1.79                     | 0.45              |
| 2:AC:90:VAL:C      | 2:AC:93:ILE:HG22  | 2.42                     | 0.45              |
| 2:AC:112:ALA:HB1   | 2:AC:199:VAL:HG23 | 1.99                     | 0.45              |
| 5:AF:1:MET:HB3     | 5:AF:65:GLU:O     | 2.16                     | 0.45              |
| 6:AG:71:THR:HA     | 6:AG:90:VAL:HG22  | 1.99                     | 0.45              |
| 6:AG:137:ARG:C     | 6:AG:141:HIS:HD1  | 2.24                     | 0.45              |
| 8:AI:46:VAL:HB     | 8:AI:79:ARG:HD3   | 1.97                     | 0.45              |
| 12:AM:16:ILE:HG23  | 12:AM:17:ALA:N    | 2.30                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:AM:21:ILE:HG22  | 12:AM:64:VAL:CG1   | 2.44                     | 0.45              |
| 15:AP:7:ALA:HB1    | 15:AP:29:ASN:CB    | 2.47                     | 0.45              |
| 18:AS:4:LEU:O      | 18:AS:6:LYS:N      | 2.49                     | 0.45              |
| 20:AB:9:LEU:CD2    | 20:AB:11:ALA:H     | 2.17                     | 0.45              |
| 22:BA:18:G:H2'     | 22:BA:19:C:C6      | 2.52                     | 0.45              |
| 23:BB:137:U:O5'    | 23:BB:137:U:H6     | 1.99                     | 0.45              |
| 23:BB:215:G:O4'    | 23:BB:216:A:H4'    | 2.17                     | 0.45              |
| 23:BB:364:C:O2'    | 23:BB:365:U:H5'    | 2.16                     | 0.45              |
| 23:BB:441:U:HO2'   | 23:BB:442:G:H5'    | 1.80                     | 0.45              |
| 23:BB:539:G:H2'    | 23:BB:540:C:H6     | 1.81                     | 0.45              |
| 23:BB:773:U:H4'    | 25:BC:47:ARG:CA    | 2.47                     | 0.45              |
| 23:BB:1125:G:H3'   | 23:BB:1126:A:H5''  | 1.98                     | 0.45              |
| 23:BB:1410:G:H2'   | 23:BB:1411:U:H6    | 1.77                     | 0.45              |
| 23:BB:1450:G:N2    | 23:BB:1452:G:H1    | 1.95                     | 0.45              |
| 23:BB:1708:C:H2'   | 23:BB:1709:U:H6    | 1.81                     | 0.45              |
| 23:BB:1885:A:H3'   | 23:BB:1886:U:C6    | 2.51                     | 0.45              |
| 23:BB:2187:U:O2    | 23:BB:2187:U:H2'   | 2.16                     | 0.45              |
| 23:BB:2710:C:H2'   | 23:BB:2711:A:H8    | 1.80                     | 0.45              |
| 23:BB:2722:G:H2'   | 23:BB:2723:C:H6    | 1.82                     | 0.45              |
| 23:BB:2751:G:OP2   | 29:BG:3:VAL:HG13   | 2.16                     | 0.45              |
| 23:BB:2780:G:C2    | 31:BJ:120:ARG:HG3  | 2.51                     | 0.45              |
| 25:BC:163:ILE:HG22 | 25:BC:172:THR:HG21 | 1.98                     | 0.45              |
| 26:BD:165:MET:HG3  | 26:BD:166:GLY:N    | 2.32                     | 0.45              |
| 26:BD:187:LEU:HD23 | 26:BD:187:LEU:C    | 2.41                     | 0.45              |
| 29:BG:35:THR:C     | 29:BG:36:LEU:HD12  | 2.42                     | 0.45              |
| 33:BL:120:VAL:CG1  | 33:BL:138:ALA:HB3  | 2.47                     | 0.45              |
| 34:BM:21:ALA:C     | 34:BM:96:ILE:HG13  | 2.42                     | 0.45              |
| 35:BN:32:GLU:O     | 35:BN:114:GLU:HA   | 2.17                     | 0.45              |
| 38:BQ:95:ALA:C     | 38:BQ:97:ILE:N     | 2.67                     | 0.45              |
| 39:BR:38:VAL:C     | 39:BR:40:MET:H     | 2.25                     | 0.45              |
| 39:BR:66:HIS:CA    | 39:BR:98:ILE:HD13  | 2.45                     | 0.45              |
| 41:BT:15:HIS:CB    | 41:BT:31:VAL:HG21  | 2.46                     | 0.45              |
| 41:BT:25:GLU:CG    | 41:BT:26:LYS:N     | 2.79                     | 0.45              |
| 42:BU:3:LYS:HD2    | 42:BU:81:ARG:NH2   | 2.31                     | 0.45              |
| 44:BX:16:THR:O     | 44:BX:20:ASN:HB2   | 2.17                     | 0.45              |
| 44:BX:22:LEU:HA    | 44:BX:47:ARG:NH2   | 2.32                     | 0.45              |
| 46:BZ:50:ASP:O     | 46:BZ:53:THR:HG22  | 2.16                     | 0.45              |
| 48:B1:42:VAL:CG1   | 48:B1:43:ARG:HE    | 2.28                     | 0.45              |
| 1:CA:12:U:H4'      | 1:CA:526:C:H4'     | 1.98                     | 0.45              |
| 1:CA:564:C:C5      | 16:CQ:32:ILE:HD11  | 2.52                     | 0.45              |
| 1:CA:613:C:H2'     | 1:CA:614:C:H6      | 1.82                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:820:U:H4'    | 1:CA:821:G:OP2     | 2.16                     | 0.45              |
| 1:CA:880:C:H2'    | 1:CA:881:G:H8      | 1.81                     | 0.45              |
| 1:CA:950:U:H2'    | 1:CA:951:G:H8      | 1.82                     | 0.45              |
| 1:CA:975:A:H2'    | 1:CA:976:G:OP2     | 2.17                     | 0.45              |
| 1:CA:1060:U:C5'   | 9:CJ:53:ILE:HG12   | 2.46                     | 0.45              |
| 1:CA:1065:U:H1'   | 1:CA:1066:C:OP2    | 2.17                     | 0.45              |
| 1:CA:1425:U:H2'   | 1:CA:1426:G:H8     | 1.82                     | 0.45              |
| 3:CD:12:ARG:C     | 3:CD:37:PRO:HG3    | 2.42                     | 0.45              |
| 4:CE:36:THR:CG2   | 4:CE:37:VAL:H      | 2.25                     | 0.45              |
| 4:CE:125:LYS:HE3  | 4:CE:127:TYR:CE1   | 2.52                     | 0.45              |
| 5:CF:22:ILE:O     | 5:CF:26:THR:HG23   | 2.16                     | 0.45              |
| 7:CH:17:GLN:HG3   | 7:CH:71:VAL:HG21   | 1.99                     | 0.45              |
| 9:CJ:40:ILE:CD1   | 9:CJ:73:LEU:HB3    | 2.46                     | 0.45              |
| 11:CL:72:ASN:ND2  | 11:CL:73:LEU:H     | 2.15                     | 0.45              |
| 13:CN:14:ALA:HA   | 13:CN:17:ASP:OD2   | 2.16                     | 0.45              |
| 20:CB:95:TRP:HZ2  | 20:CB:100:LEU:HD13 | 1.81                     | 0.45              |
| 22:DA:57:A:H2     | 28:DF:29:ARG:HH22  | 1.61                     | 0.45              |
| 22:DA:66:A:O2'    | 22:DA:67:G:C5'     | 2.61                     | 0.45              |
| 23:DB:38:A:H1'    | 27:DE:43:THR:O     | 2.17                     | 0.45              |
| 23:DB:324:A:H61   | 23:DB:338:G:C2'    | 2.30                     | 0.45              |
| 23:DB:544:C:O2'   | 23:DB:545:U:O4'    | 2.34                     | 0.45              |
| 23:DB:1199:U:C2   | 23:DB:1200:C:C6    | 3.05                     | 0.45              |
| 23:DB:1790:C:H2'  | 23:DB:1791:A:C8    | 2.52                     | 0.45              |
| 23:DB:2340:A:H2'  | 23:DB:2341:G:H8    | 1.81                     | 0.45              |
| 23:DB:2363:G:O2'  | 23:DB:2364:C:H5'   | 2.16                     | 0.45              |
| 23:DB:2684:U:H4'  | 32:DK:76:VAL:CG2   | 2.43                     | 0.45              |
| 23:DB:2835:A:H61  | 23:DB:2878:U:H2'   | 1.80                     | 0.45              |
| 23:DB:2886:A:C2   | 23:DB:2887:A:N7    | 2.85                     | 0.45              |
| 26:DD:23:PRO:HB3  | 26:DD:188:LEU:HG   | 1.97                     | 0.45              |
| 28:DF:35:LEU:HD23 | 28:DF:153:ILE:HG12 | 1.99                     | 0.45              |
| 30:DH:122:LEU:CD1 | 30:DH:146:VAL:HG22 | 2.41                     | 0.45              |
| 33:DL:78:ARG:HA   | 33:DL:113:ALA:HB2  | 1.97                     | 0.45              |
| 34:DM:81:ARG:NH1  | 34:DM:81:ARG:HB2   | 2.32                     | 0.45              |
| 37:DP:111:GLU:C   | 37:DP:113:LEU:N    | 2.74                     | 0.45              |
| 39:DR:89:HIS:O    | 39:DR:90:ARG:CG    | 2.57                     | 0.45              |
| 43:DW:47:GLY:HA2  | 43:DW:71:LYS:O     | 2.16                     | 0.45              |
| 45:DY:6:ILE:HD11  | 45:DY:35:VAL:CB    | 2.47                     | 0.45              |
| 47:D0:43:THR:O    | 47:D0:44:ALA:HB3   | 2.16                     | 0.45              |
| 52:DI:53:PRO:HG2  | 52:DI:77:VAL:HG11  | 1.98                     | 0.45              |
| 1:AA:36:C:H2'     | 1:AA:37:U:O4'      | 2.17                     | 0.45              |
| 1:AA:89:U:O2'     | 1:AA:90:C:O5'      | 2.33                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:731:G:OP1     | 1:AA:766:A:H1'     | 2.17                     | 0.45              |
| 1:AA:796:C:H4'     | 10:AK:126:ARG:HH21 | 1.82                     | 0.45              |
| 1:AA:847:G:H2'     | 1:AA:848:C:H6      | 1.82                     | 0.45              |
| 2:AC:8:GLY:HA2     | 2:AC:11:LEU:CG     | 2.43                     | 0.45              |
| 2:AC:156:LEU:H     | 2:AC:156:LEU:CD1   | 2.11                     | 0.45              |
| 2:AC:185:THR:HG22  | 2:AC:186:SER:N     | 2.26                     | 0.45              |
| 3:AD:172:VAL:HA    | 3:AD:178:GLU:O     | 2.16                     | 0.45              |
| 7:AH:54:THR:HG23   | 7:AH:55:LYS:HG2    | 1.99                     | 0.45              |
| 16:AQ:56:ASP:C     | 16:AQ:79:GLU:HB3   | 2.40                     | 0.45              |
| 19:AT:17:ARG:C     | 19:AT:17:ARG:HD2   | 2.42                     | 0.45              |
| 20:AB:186:VAL:CG2  | 20:AB:198:VAL:HG23 | 2.47                     | 0.45              |
| 22:BA:94:A:H2'     | 22:BA:95:U:O4'     | 2.17                     | 0.45              |
| 22:BA:99:A:N3      | 22:BA:99:A:H2'     | 2.32                     | 0.45              |
| 23:BB:37:C:C2'     | 27:BE:46:GLN:CG    | 2.77                     | 0.45              |
| 23:BB:340:A:H2'    | 23:BB:341:C:C5'    | 2.47                     | 0.45              |
| 23:BB:350:G:H2'    | 23:BB:351:C:H6     | 1.82                     | 0.45              |
| 23:BB:515:A:H3'    | 23:BB:516:C:H6     | 1.80                     | 0.45              |
| 23:BB:829:A:H4'    | 55:BB:3324:HOH:O   | 2.16                     | 0.45              |
| 23:BB:1275:A:N3    | 23:BB:1275:A:C3'   | 2.78                     | 0.45              |
| 23:BB:2045:C:H5''  | 47:B0:14:MET:HE3   | 1.97                     | 0.45              |
| 23:BB:2759:G:H21   | 29:BG:138:GLN:HE22 | 1.64                     | 0.45              |
| 25:BC:50:THR:C     | 25:BC:51:ARG:HG3   | 2.42                     | 0.45              |
| 25:BC:140:VAL:CG1  | 25:BC:163:ILE:HD11 | 2.46                     | 0.45              |
| 25:BC:237:ARG:C    | 25:BC:237:ARG:HE   | 2.25                     | 0.45              |
| 26:BD:52:THR:HG22  | 26:BD:75:ALA:CB    | 2.44                     | 0.45              |
| 27:BE:57:LYS:HA    | 27:BE:57:LYS:CE    | 2.47                     | 0.45              |
| 27:BE:176:ASP:CG   | 27:BE:177:PRO:HD2  | 2.41                     | 0.45              |
| 30:BH:24:GLY:HA2   | 30:BH:27:ARG:HH12  | 1.81                     | 0.45              |
| 30:BH:39:ALA:O     | 30:BH:44:ILE:HD11  | 2.17                     | 0.45              |
| 30:BH:94:ILE:HA    | 30:BH:98:ASP:OD2   | 2.17                     | 0.45              |
| 31:BJ:93:ILE:CD1   | 31:BJ:100:VAL:HG11 | 2.46                     | 0.45              |
| 32:BK:28:SER:O     | 32:BK:29:HIS:HB2   | 2.17                     | 0.45              |
| 33:BL:60:ARG:HD2   | 50:B3:7:ARG:CZ     | 2.47                     | 0.45              |
| 33:BL:122:VAL:HG23 | 33:BL:140:GLY:O    | 2.16                     | 0.45              |
| 35:BN:41:ALA:C     | 35:BN:43:GLU:H     | 2.24                     | 0.45              |
| 37:BP:15:ASP:OD1   | 37:BP:15:ASP:N     | 2.49                     | 0.45              |
| 37:BP:114:ASN:N    | 37:BP:114:ASN:ND2  | 2.61                     | 0.45              |
| 38:BQ:33:VAL:CG1   | 38:BQ:34:ALA:H     | 2.14                     | 0.45              |
| 38:BQ:61:ILE:HB    | 38:BQ:75:TYR:CZ    | 2.52                     | 0.45              |
| 39:BR:16:GLU:HG3   | 39:BR:17:GLY:H     | 1.82                     | 0.45              |
| 40:BS:31:GLN:HB3   | 40:BS:35:ILE:HG22  | 1.99                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:BT:61:LEU:CD1   | 41:BT:62:VAL:H     | 2.28                     | 0.45              |
| 42:BU:44:HIS:HB2   | 42:BU:56:GLY:H     | 1.80                     | 0.45              |
| 45:BY:3:THR:O      | 45:BY:6:ILE:HG23   | 2.17                     | 0.45              |
| 49:B2:18:PHE:HB3   | 49:B2:19:ARG:H     | 1.51                     | 0.45              |
| 1:CA:404:G:H2'     | 1:CA:405:U:C6      | 2.52                     | 0.45              |
| 1:CA:451:A:OP2     | 15:CP:70:ARG:NH2   | 2.50                     | 0.45              |
| 1:CA:551:U:O2'     | 1:CA:552:U:H5'     | 2.17                     | 0.45              |
| 1:CA:611:C:H2'     | 1:CA:612:C:H6      | 1.80                     | 0.45              |
| 1:CA:902:G:H2'     | 1:CA:903:G:C8      | 2.51                     | 0.45              |
| 1:CA:1102:A:O2'    | 1:CA:1103:C:H5'    | 2.17                     | 0.45              |
| 1:CA:1130:A:H2'    | 1:CA:1131:G:H8     | 1.81                     | 0.45              |
| 1:CA:1158:C:O2'    | 20:CB:131:LYS:HD3  | 2.16                     | 0.45              |
| 1:CA:1453:G:H2'    | 1:CA:1454:G:O4'    | 2.17                     | 0.45              |
| 2:CC:8:GLY:C       | 2:CC:11:LEU:HG     | 2.41                     | 0.45              |
| 2:CC:59:PRO:CG     | 2:CC:62:SER:HB2    | 2.33                     | 0.45              |
| 2:CC:177:LEU:HD22  | 2:CC:177:LEU:H     | 1.81                     | 0.45              |
| 3:CD:54:LEU:C      | 3:CD:54:LEU:HD13   | 2.41                     | 0.45              |
| 3:CD:141:VAL:O     | 3:CD:141:VAL:HG23  | 2.16                     | 0.45              |
| 5:CF:62:MET:HG3    | 5:CF:64:VAL:CG2    | 2.42                     | 0.45              |
| 8:CI:26:LYS:HG3    | 8:CI:61:ASP:HB2    | 1.97                     | 0.45              |
| 10:CK:69:CYS:O     | 10:CK:73:VAL:N     | 2.49                     | 0.45              |
| 11:CL:79:ILE:C     | 11:CL:101:LEU:HD12 | 2.41                     | 0.45              |
| 18:CS:39:ILE:HB    | 18:CS:66:VAL:HA    | 1.98                     | 0.45              |
| 23:DB:476:G:N2     | 23:DB:478:A:H3'    | 2.32                     | 0.45              |
| 23:DB:483:A:C2'    | 23:DB:484:C:H5'    | 2.43                     | 0.45              |
| 23:DB:633:A:H2'    | 23:DB:634:C:O4'    | 2.16                     | 0.45              |
| 23:DB:730:A:C4'    | 25:DC:16:VAL:HG13  | 2.47                     | 0.45              |
| 23:DB:747:U:O3'    | 40:DS:89:ALA:HB3   | 2.17                     | 0.45              |
| 23:DB:844:A:C2     | 23:DB:845:A:N1     | 2.84                     | 0.45              |
| 23:DB:1175:A:H2'   | 23:DB:1176:U:C5'   | 2.42                     | 0.45              |
| 23:DB:1700:A:C2'   | 23:DB:1701:A:H5'   | 2.44                     | 0.45              |
| 23:DB:1760:C:H2'   | 23:DB:1761:C:O4'   | 2.16                     | 0.45              |
| 23:DB:1773:A:C8    | 23:DB:1829:A:C8    | 3.05                     | 0.45              |
| 23:DB:1796:U:O3'   | 25:DC:251:THR:HA   | 2.16                     | 0.45              |
| 23:DB:2259:U:C6    | 23:DB:2427:C:C5    | 3.05                     | 0.45              |
| 23:DB:2420:C:C5    | 50:D3:30:HIS:O     | 2.70                     | 0.45              |
| 25:DC:63:ILE:CG2   | 25:DC:64:VAL:N     | 2.79                     | 0.45              |
| 25:DC:163:ILE:HG22 | 25:DC:164:VAL:N    | 2.32                     | 0.45              |
| 26:DD:90:PHE:C     | 26:DD:92:VAL:H     | 2.23                     | 0.45              |
| 26:DD:186:LEU:HD11 | 37:DP:5:LYS:HE2    | 1.98                     | 0.45              |
| 27:DE:149:ILE:HD11 | 27:DE:187:VAL:N    | 2.31                     | 0.45              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 29:DG:71:LEU:O     | 29:DG:74:MET:HB2  | 2.16                     | 0.45              |
| 31:DJ:14:ASP:HB3   | 31:DJ:16:TYR:CD1  | 2.52                     | 0.45              |
| 32:DK:71:ARG:HB3   | 32:DK:72:PRO:CD   | 2.46                     | 0.45              |
| 33:DL:118:THR:HG23 | 33:DL:119:PRO:HD3 | 1.97                     | 0.45              |
| 36:DO:18:LEU:CD1   | 43:DW:76:ARG:HH21 | 2.29                     | 0.45              |
| 37:DP:83:ILE:H     | 37:DP:83:ILE:HG13 | 1.51                     | 0.45              |
| 38:DQ:86:SER:C     | 38:DQ:88:GLU:H    | 2.24                     | 0.45              |
| 38:DQ:87:VAL:CG2   | 39:DR:54:VAL:HG11 | 2.46                     | 0.45              |
| 39:DR:76:LYS:HA    | 39:DR:91:GLN:N    | 2.31                     | 0.45              |
| 40:DS:1:MET:HB3    | 40:DS:4:ILE:HD12  | 1.98                     | 0.45              |
| 40:DS:10:ALA:O     | 40:DS:11:ARG:HB3  | 2.17                     | 0.45              |
| 42:DU:82:VAL:HB    | 42:DU:94:PHE:CB   | 2.43                     | 0.45              |
| 43:DW:77:LYS:C     | 43:DW:79:ILE:H    | 2.24                     | 0.45              |
| 44:DX:26:PHE:HA    | 44:DX:29:ARG:HD2  | 1.97                     | 0.45              |
| 46:DZ:54:GLY:H     | 46:DZ:57:VAL:CG2  | 2.14                     | 0.45              |
| 48:D1:31:GLU:HG2   | 48:D1:32:LYS:HG3  | 1.98                     | 0.45              |
| 1:AA:81:A:N3       | 1:AA:82:G:N7      | 2.65                     | 0.45              |
| 1:AA:238:A:C3'     | 1:AA:239:U:H5''   | 2.47                     | 0.45              |
| 1:AA:404:G:H2'     | 1:AA:405:U:C6     | 2.52                     | 0.45              |
| 1:AA:607:A:H2'     | 1:AA:608:A:C8     | 2.52                     | 0.45              |
| 1:AA:740:U:O3'     | 14:AO:38:LEU:HD21 | 2.16                     | 0.45              |
| 1:AA:1522:U:O2'    | 1:AA:1523:G:H5'   | 2.16                     | 0.45              |
| 2:AC:51:VAL:HA     | 2:AC:69:THR:HB    | 1.99                     | 0.45              |
| 3:AD:99:ASN:HD21   | 3:AD:110:ARG:HE   | 1.64                     | 0.45              |
| 3:AD:176:LYS:O     | 3:AD:177:MET:C    | 2.59                     | 0.45              |
| 6:AG:59:GLU:O      | 6:AG:63:VAL:HG23  | 2.17                     | 0.45              |
| 8:AI:61:ASP:C      | 8:AI:62:LEU:HD22  | 2.41                     | 0.45              |
| 9:AJ:68:ARG:HB3    | 9:AJ:70:HIS:NE2   | 2.32                     | 0.45              |
| 11:AL:35:ARG:HG3   | 11:AL:36:VAL:N    | 2.27                     | 0.45              |
| 12:AM:77:LYS:HE3   | 12:AM:81:ASP:HB3  | 1.99                     | 0.45              |
| 15:AP:22:ALA:HB2   | 15:AP:32:PHE:HB3  | 1.98                     | 0.45              |
| 22:BA:22:U:H2'     | 22:BA:23:G:C8     | 2.51                     | 0.45              |
| 22:BA:109:A:H2'    | 22:BA:110:C:C6    | 2.51                     | 0.45              |
| 23:BB:85:G:H5''    | 42:BU:28:LEU:HD23 | 1.99                     | 0.45              |
| 23:BB:481:G:OP2    | 42:BU:43:LYS:HG3  | 2.16                     | 0.45              |
| 23:BB:741:U:H2'    | 23:BB:742:A:H8    | 1.80                     | 0.45              |
| 23:BB:997:G:O2'    | 23:BB:998:C:H5'   | 2.17                     | 0.45              |
| 23:BB:1019:U:O2'   | 23:BB:1021:A:C2   | 2.64                     | 0.45              |
| 23:BB:1057:A:C8    | 23:BB:1086:A:C8   | 3.05                     | 0.45              |
| 23:BB:1184:U:H2'   | 23:BB:1185:G:C8   | 2.52                     | 0.45              |
| 23:BB:1601:G:O2'   | 23:BB:1602:U:H5'  | 2.16                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:BB:2340:A:H2'   | 23:BB:2341:G:H8   | 1.82                     | 0.45              |
| 23:BB:2772:C:H2'   | 23:BB:2773:C:H6   | 1.81                     | 0.45              |
| 23:BB:2821:A:H2'   | 23:BB:2822:G:H8   | 1.82                     | 0.45              |
| 24:BV:72:VAL:HA    | 24:BV:94:ALA:H    | 1.81                     | 0.45              |
| 24:BV:83:LYS:O     | 24:BV:85:LYS:N    | 2.49                     | 0.45              |
| 26:BD:13:ARG:HB2   | 26:BD:21:SER:CB   | 2.46                     | 0.45              |
| 26:BD:26:VAL:HG23  | 26:BD:26:VAL:O    | 2.17                     | 0.45              |
| 26:BD:70:LYS:HA    | 26:BD:70:LYS:CE   | 2.37                     | 0.45              |
| 28:BF:148:VAL:O    | 28:BF:150:GLY:N   | 2.50                     | 0.45              |
| 30:BH:21:VAL:HG13  | 30:BH:22:LYS:O    | 2.16                     | 0.45              |
| 30:BH:121:VAL:HG21 | 30:BH:128:HIS:NE2 | 2.31                     | 0.45              |
| 31:BJ:45:THR:HB    | 38:BQ:63:ARG:CZ   | 2.46                     | 0.45              |
| 34:BM:68:PHE:HA    | 34:BM:69:PRO:HD2  | 1.76                     | 0.45              |
| 35:BN:22:ARG:NH1   | 35:BN:69:ARG:HA   | 2.32                     | 0.45              |
| 36:BO:41:ALA:H     | 36:BO:48:LEU:HB3  | 1.81                     | 0.45              |
| 37:BP:105:LYS:HG3  | 37:BP:107:ALA:H   | 1.81                     | 0.45              |
| 38:BQ:39:ILE:CG2   | 39:BR:80:ARG:HD3  | 2.47                     | 0.45              |
| 39:BR:35:PHE:HB2   | 39:BR:64:VAL:CG2  | 2.47                     | 0.45              |
| 39:BR:62:GLU:N     | 39:BR:62:GLU:OE1  | 2.49                     | 0.45              |
| 41:BT:9:LYS:HG2    | 44:BX:22:LEU:HD11 | 1.99                     | 0.45              |
| 41:BT:29:THR:O     | 41:BT:30:ILE:HD12 | 2.17                     | 0.45              |
| 41:BT:66:LYS:O     | 41:BT:67:VAL:HB   | 2.17                     | 0.45              |
| 45:BY:37:ARG:HH11  | 45:BY:37:ARG:HG3  | 1.82                     | 0.45              |
| 47:B0:28:SER:HB2   | 47:B0:34:GLY:H    | 1.78                     | 0.45              |
| 47:B0:42:ILE:HG21  | 47:B0:47:TYR:CE1  | 2.51                     | 0.45              |
| 51:B4:13:ASN:N     | 51:B4:13:ASN:ND2  | 2.63                     | 0.45              |
| 1:CA:334:C:H2'     | 1:CA:335:C:H6     | 1.81                     | 0.45              |
| 1:CA:975:A:OP2     | 1:CA:975:A:H4'    | 2.16                     | 0.45              |
| 1:CA:1136:C:O5'    | 1:CA:1136:C:H6    | 2.00                     | 0.45              |
| 1:CA:1288:A:N1     | 1:CA:1371:G:H1'   | 2.31                     | 0.45              |
| 1:CA:1387:G:H2'    | 1:CA:1388:C:H6    | 1.79                     | 0.45              |
| 1:CA:1451:U:C5'    | 1:CA:1452:C:OP2   | 2.59                     | 0.45              |
| 1:CA:1516:G:N1     | 1:CA:1519:A:OP2   | 2.50                     | 0.45              |
| 2:CC:41:TYR:CD2    | 2:CC:41:TYR:N     | 2.83                     | 0.45              |
| 4:CE:110:MET:O     | 4:CE:114:LEU:HG   | 2.16                     | 0.45              |
| 8:CI:120:ALA:O     | 8:CI:121:ARG:HG2  | 2.17                     | 0.45              |
| 11:CL:13:ARG:O     | 11:CL:14:LYS:HB3  | 2.16                     | 0.45              |
| 14:CO:69:LEU:HD12  | 14:CO:77:TYR:N    | 2.31                     | 0.45              |
| 15:CP:48:GLU:HG2   | 15:CP:50:THR:H    | 1.81                     | 0.45              |
| 20:CB:34:ARG:NE    | 20:CB:39:ILE:HG13 | 2.32                     | 0.45              |
| 21:CU:16:ARG:HA    | 21:CU:19:LYS:HZ3  | 1.82                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:CU:33:ARG:HB3  | 21:CU:34:ARG:H    | 1.65                     | 0.45              |
| 23:DB:38:A:N3     | 27:DE:43:THR:HG22 | 2.32                     | 0.45              |
| 23:DB:40:U:H2'    | 23:DB:41:C:C6     | 2.52                     | 0.45              |
| 23:DB:99:U:O2     | 23:DB:99:U:O4'    | 2.33                     | 0.45              |
| 23:DB:257:C:H3'   | 23:DB:258:G:H8    | 1.82                     | 0.45              |
| 23:DB:259:G:O2'   | 23:DB:260:G:H5'   | 2.16                     | 0.45              |
| 23:DB:437:U:O2'   | 23:DB:438:G:H5'   | 2.16                     | 0.45              |
| 23:DB:904:G:H2'   | 23:DB:905:A:H8    | 1.82                     | 0.45              |
| 23:DB:1076:C:O2'  | 23:DB:1077:A:H5'  | 2.17                     | 0.45              |
| 23:DB:1791:A:N1   | 23:DB:1829:A:H5'  | 2.31                     | 0.45              |
| 23:DB:1803:A:H2   | 23:DB:1823:G:C1'  | 2.29                     | 0.45              |
| 23:DB:1821:A:H5'  | 25:DC:155:ARG:NH2 | 2.28                     | 0.45              |
| 23:DB:1843:C:H2'  | 23:DB:1844:C:H6   | 1.81                     | 0.45              |
| 23:DB:2188:U:H2'  | 23:DB:2189:U:O4'  | 2.16                     | 0.45              |
| 23:DB:2464:G:H2'  | 23:DB:2465:C:C6   | 2.52                     | 0.45              |
| 23:DB:2685:G:OP1  | 37:DP:62:LYS:NZ   | 2.47                     | 0.45              |
| 23:DB:2884:U:C2   | 47:D0:48:TYR:CZ   | 3.04                     | 0.45              |
| 25:DC:130:PRO:HA  | 25:DC:188:ARG:HA  | 1.98                     | 0.45              |
| 25:DC:156:SER:O   | 25:DC:194:VAL:O   | 2.35                     | 0.45              |
| 27:DE:135:ALA:O   | 27:DE:139:LYS:HB3 | 2.16                     | 0.45              |
| 38:DQ:101:ASP:OD1 | 38:DQ:104:ALA:HB3 | 2.17                     | 0.45              |
| 39:DR:44:GLY:N    | 39:DR:53:PHE:CE2  | 2.84                     | 0.45              |
| 39:DR:69:GLY:HA2  | 39:DR:97:LYS:N    | 2.29                     | 0.45              |
| 42:DU:3:LYS:O     | 42:DU:4:ILE:HB    | 2.17                     | 0.45              |
| 48:D1:8:ILE:CG2   | 48:D1:27:ARG:HD3  | 2.46                     | 0.45              |
| 51:D4:10:LEU:HD12 | 51:D4:10:LEU:N    | 2.32                     | 0.45              |
| 52:DI:89:SER:HA   | 52:DI:97:VAL:CG1  | 2.47                     | 0.45              |
| 1:AA:24:U:O2'     | 1:AA:25:C:H5'     | 2.16                     | 0.45              |
| 1:AA:182:A:O2'    | 1:AA:183:C:O5'    | 2.34                     | 0.45              |
| 1:AA:402:G:H2'    | 1:AA:403:C:C6     | 2.52                     | 0.45              |
| 1:AA:662:U:H2'    | 1:AA:663:A:H8     | 1.76                     | 0.45              |
| 1:AA:1399:C:H1'   | 55:AA:1970:HOH:O  | 2.16                     | 0.45              |
| 1:AA:1515:G:O2'   | 1:AA:1516:G:H5'   | 2.17                     | 0.45              |
| 2:AC:5:HIS:O      | 2:AC:9:ILE:HG22   | 2.16                     | 0.45              |
| 2:AC:153:SER:CB   | 2:AC:196:GLY:H    | 2.27                     | 0.45              |
| 8:AI:57:VAL:C     | 8:AI:59:LYS:H     | 2.25                     | 0.45              |
| 11:AL:17:LYS:HE3  | 11:AL:17:LYS:HB2  | 1.82                     | 0.45              |
| 12:AM:8:ILE:O     | 12:AM:8:ILE:HG13  | 2.17                     | 0.45              |
| 13:AN:81:ILE:HD12 | 13:AN:82:LYS:N    | 2.31                     | 0.45              |
| 18:AS:29:PRO:CA   | 18:AS:47:THR:HB   | 2.47                     | 0.45              |
| 20:AB:140:LEU:HB3 | 20:AB:144:GLU:OE2 | 2.17                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:BA:78:A:O2'     | 22:BA:79:G:H5'    | 2.17                     | 0.45              |
| 23:BB:139:U:C2     | 41:BT:1:MET:HG2   | 2.51                     | 0.45              |
| 23:BB:992:C:H2'    | 23:BB:993:G:C8    | 2.51                     | 0.45              |
| 23:BB:1100:C:H2'   | 23:BB:1101:U:H6   | 1.81                     | 0.45              |
| 23:BB:1322:A:H2'   | 23:BB:1323:C:H5'  | 1.98                     | 0.45              |
| 23:BB:1509:A:C5'   | 23:BB:1510:G:H5'  | 2.47                     | 0.45              |
| 23:BB:1683:U:H2'   | 23:BB:1684:G:C8   | 2.51                     | 0.45              |
| 23:BB:1987:A:H2'   | 23:BB:1988:G:H8   | 1.82                     | 0.45              |
| 23:BB:2465:C:O2'   | 23:BB:2466:C:H5'  | 2.16                     | 0.45              |
| 23:BB:2708:G:H4'   | 35:BN:68:ALA:HB1  | 1.99                     | 0.45              |
| 23:BB:2830:C:O2'   | 23:BB:2831:G:H5'  | 2.17                     | 0.45              |
| 25:BC:153:LEU:H    | 25:BC:153:LEU:CD2 | 2.26                     | 0.45              |
| 26:BD:26:VAL:O     | 26:BD:27:ILE:C    | 2.60                     | 0.45              |
| 26:BD:128:ARG:NH1  | 26:BD:144:GLY:HA2 | 2.32                     | 0.45              |
| 27:BE:7:ASP:O      | 27:BE:8:ALA:HB3   | 2.17                     | 0.45              |
| 30:BH:2:GLN:HE22   | 30:BH:20:ASN:N    | 2.14                     | 0.45              |
| 30:BH:19:VAL:O     | 30:BH:20:ASN:C    | 2.59                     | 0.45              |
| 30:BH:32:PRO:C     | 30:BH:34:GLY:H    | 2.24                     | 0.45              |
| 30:BH:50:ARG:O     | 30:BH:50:ARG:HG2  | 2.15                     | 0.45              |
| 31:BJ:118:MET:O    | 31:BJ:119:PHE:C   | 2.59                     | 0.45              |
| 31:BJ:128:ASN:CG   | 31:BJ:129:GLU:N   | 2.72                     | 0.45              |
| 35:BN:73:ASN:HA    | 35:BN:76:VAL:CG1  | 2.46                     | 0.45              |
| 37:BP:28:LYS:HG2   | 37:BP:44:GLY:C    | 2.41                     | 0.45              |
| 38:BQ:73:ILE:HG13  | 38:BQ:77:LYS:HD2  | 1.99                     | 0.45              |
| 38:BQ:103:VAL:HG23 | 38:BQ:104:ALA:N   | 2.31                     | 0.45              |
| 43:BW:24:ARG:HB3   | 43:BW:57:THR:O    | 2.16                     | 0.45              |
| 52:BI:38:CYS:O     | 52:BI:42:ASN:ND2  | 2.49                     | 0.45              |
| 1:CA:239:U:H6      | 1:CA:239:U:H5'    | 1.80                     | 0.45              |
| 1:CA:1098:C:O2'    | 1:CA:1099:G:H5'   | 2.16                     | 0.45              |
| 1:CA:1128:C:H4'    | 1:CA:1148:U:O2    | 2.17                     | 0.45              |
| 1:CA:1227:A:H4'    | 12:CM:113:LYS:HE2 | 1.97                     | 0.45              |
| 1:CA:1382:C:H5'    | 6:CG:78:ARG:HE    | 1.82                     | 0.45              |
| 1:CA:1488:G:H2'    | 1:CA:1489:G:H8    | 1.82                     | 0.45              |
| 2:CC:10:ARG:HH11   | 2:CC:10:ARG:HG2   | 1.82                     | 0.45              |
| 4:CE:82:HIS:NE2    | 4:CE:146:MET:HB2  | 2.31                     | 0.45              |
| 11:CL:82:ARG:HB2   | 11:CL:97:VAL:HG13 | 1.98                     | 0.45              |
| 14:CO:63:ARG:HH21  | 14:CO:87:ARG:NH1  | 2.15                     | 0.45              |
| 16:CQ:60:ILE:HG22  | 16:CQ:74:LEU:HA   | 1.98                     | 0.45              |
| 18:CS:3:SER:C      | 18:CS:4:LEU:HD12  | 2.42                     | 0.45              |
| 20:CB:211:LEU:HG   | 20:CB:212:TYR:N   | 2.32                     | 0.45              |
| 22:DA:6:G:O2'      | 22:DA:7:G:H5'     | 2.16                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:97:C:H2'    | 23:DB:98:G:O4'     | 2.17                     | 0.45              |
| 23:DB:510:C:O2'   | 23:DB:1236:G:H5'   | 2.17                     | 0.45              |
| 23:DB:544:C:H2'   | 23:DB:545:U:C2     | 2.52                     | 0.45              |
| 23:DB:547:A:N3    | 23:DB:547:A:C2'    | 2.77                     | 0.45              |
| 23:DB:1286:A:H1'  | 23:DB:1288:G:OP2   | 2.17                     | 0.45              |
| 23:DB:1820:U:N3   | 25:DC:197:ALA:HB1  | 2.27                     | 0.45              |
| 23:DB:2144:G:C2   | 23:DB:2146:C:H5'   | 2.52                     | 0.45              |
| 23:DB:2651:C:O2'  | 23:DB:2652:C:H5'   | 2.17                     | 0.45              |
| 23:DB:2673:G:H2'  | 23:DB:2674:G:C8    | 2.52                     | 0.45              |
| 25:DC:50:THR:O    | 25:DC:51:ARG:C     | 2.59                     | 0.45              |
| 25:DC:86:ARG:HB2  | 25:DC:86:ARG:HH11  | 1.81                     | 0.45              |
| 25:DC:259:ASN:O   | 25:DC:261:ARG:HG3  | 2.17                     | 0.45              |
| 28:DF:7:TYR:HA    | 28:DF:11:VAL:HB    | 1.98                     | 0.45              |
| 29:DG:100:ASN:HA  | 29:DG:116:LEU:HD11 | 1.99                     | 0.45              |
| 29:DG:103:ASN:HA  | 29:DG:112:VAL:O    | 2.17                     | 0.45              |
| 29:DG:141:GLY:O   | 29:DG:144:ALA:HB3  | 2.16                     | 0.45              |
| 31:DJ:73:VAL:HA   | 31:DJ:88:THR:O     | 2.17                     | 0.45              |
| 33:DL:92:LEU:HB2  | 33:DL:125:LEU:HD11 | 1.99                     | 0.45              |
| 34:DM:33:LEU:HD21 | 34:DM:124:LEU:HD13 | 1.98                     | 0.45              |
| 36:DO:4:LYS:HD2   | 36:DO:4:LYS:C      | 2.41                     | 0.45              |
| 36:DO:98:GLN:O    | 36:DO:99:TYR:HB2   | 2.17                     | 0.45              |
| 40:DS:36:LEU:HA   | 40:DS:39:THR:CG2   | 2.47                     | 0.45              |
| 41:DT:49:LYS:O    | 41:DT:51:PHE:N     | 2.41                     | 0.45              |
| 42:DU:27:VAL:CB   | 42:DU:33:VAL:HG22  | 2.46                     | 0.45              |
| 44:DX:17:GLU:HA   | 44:DX:21:LEU:CB    | 2.46                     | 0.45              |
| 52:DI:99:LYS:HB2  | 52:DI:140:GLU:OE1  | 2.16                     | 0.45              |
| 1:AA:202:G:N2     | 1:AA:465:A:H61     | 2.14                     | 0.45              |
| 1:AA:295:C:H2'    | 1:AA:296:U:C6      | 2.52                     | 0.45              |
| 1:AA:408:A:OP1    | 3:AD:111:ALA:HB3   | 2.17                     | 0.45              |
| 1:AA:543:U:P      | 3:AD:13:ARG:HH21   | 2.40                     | 0.45              |
| 1:AA:1096:C:H2'   | 1:AA:1097:C:C6     | 2.52                     | 0.45              |
| 1:AA:1250:A:O2'   | 1:AA:1251:A:H5'    | 2.17                     | 0.45              |
| 1:AA:1314:C:H5    | 18:AS:5:LYS:HZ3    | 1.61                     | 0.45              |
| 1:AA:1380:U:C4    | 6:AG:2:ARG:HG3     | 2.52                     | 0.45              |
| 5:AF:66:ALA:HB1   | 5:AF:67:PRO:HD2    | 1.99                     | 0.45              |
| 10:AK:80:ASN:HD21 | 10:AK:107:THR:HG23 | 1.82                     | 0.45              |
| 11:AL:30:ARG:HH11 | 11:AL:30:ARG:CB    | 2.29                     | 0.45              |
| 11:AL:52:CYS:SG   | 11:AL:66:ILE:HD11  | 2.56                     | 0.45              |
| 12:AM:44:ILE:CA   | 12:AM:47:LEU:HD13  | 2.47                     | 0.45              |
| 13:AN:60:ARG:HE   | 13:AN:62:ARG:CZ    | 2.30                     | 0.45              |
| 15:AP:4:ILE:HA    | 15:AP:20:VAL:O     | 2.16                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:AP:60:TRP:C     | 15:AP:65:ALA:HB3   | 2.42                     | 0.45              |
| 16:AQ:23:ALA:HB1   | 16:AQ:40:THR:CG2   | 2.47                     | 0.45              |
| 23:BB:15:G:H4'     | 47:B0:17:SER:OG    | 2.17                     | 0.45              |
| 23:BB:143:C:C3'    | 23:BB:144:A:C8     | 3.00                     | 0.45              |
| 23:BB:338:G:C2     | 23:BB:339:U:C1'    | 2.99                     | 0.45              |
| 23:BB:402:A:H2'    | 23:BB:403:U:O4'    | 2.16                     | 0.45              |
| 23:BB:463:G:N2     | 23:BB:466:A:OP2    | 2.48                     | 0.45              |
| 23:BB:527:C:H5'    | 55:BB:3419:HOH:O   | 2.17                     | 0.45              |
| 23:BB:811:U:C6     | 33:BL:29:LYS:HD3   | 2.52                     | 0.45              |
| 23:BB:1255:U:H2'   | 27:BE:67:ARG:HB3   | 1.99                     | 0.45              |
| 23:BB:1309:G:H4'   | 49:B2:7:PRO:CG     | 2.45                     | 0.45              |
| 23:BB:1547:C:H2'   | 23:BB:1548:A:C8    | 2.52                     | 0.45              |
| 23:BB:1669:A:H2'   | 23:BB:1669:A:N3    | 2.30                     | 0.45              |
| 23:BB:1752:C:H4'   | 23:BB:2862:G:OP1   | 2.16                     | 0.45              |
| 23:BB:2291:U:H2'   | 23:BB:2292:U:H6    | 1.80                     | 0.45              |
| 23:BB:2319:G:C2    | 23:BB:2321:U:O4    | 2.70                     | 0.45              |
| 23:BB:2651:C:O2'   | 23:BB:2652:C:H5'   | 2.17                     | 0.45              |
| 23:BB:2673:G:H2'   | 23:BB:2674:G:C8    | 2.52                     | 0.45              |
| 23:BB:2776:A:H4'   | 23:BB:2777:G:C5'   | 2.46                     | 0.45              |
| 26:BD:38:LYS:HG2   | 26:BD:39:ASP:N     | 2.22                     | 0.45              |
| 26:BD:148:GLN:HB3  | 26:BD:151:THR:HG21 | 1.98                     | 0.45              |
| 28:BF:31:GLU:HB3   | 28:BF:32:LYS:H     | 1.54                     | 0.45              |
| 28:BF:135:ILE:HG23 | 28:BF:136:ILE:N    | 2.31                     | 0.45              |
| 29:BG:120:ILE:HD12 | 29:BG:120:ILE:N    | 2.32                     | 0.45              |
| 29:BG:121:THR:O    | 29:BG:133:LYS:HD3  | 2.16                     | 0.45              |
| 30:BH:11:ASN:HD22  | 30:BH:12:LEU:N     | 2.10                     | 0.45              |
| 32:BK:8:LEU:HB3    | 32:BK:84:CYS:SG    | 2.57                     | 0.45              |
| 32:BK:10:VAL:HG13  | 32:BK:19:VAL:CG2   | 2.46                     | 0.45              |
| 33:BL:33:ARG:NH1   | 33:BL:34:GLY:HA3   | 2.32                     | 0.45              |
| 33:BL:60:ARG:HD3   | 50:B3:11:LYS:NZ    | 2.31                     | 0.45              |
| 33:BL:76:GLU:O     | 33:BL:77:ILE:C     | 2.60                     | 0.45              |
| 34:BM:109:PRO:O    | 34:BM:112:LEU:HB2  | 2.17                     | 0.45              |
| 35:BN:101:GLY:H    | 35:BN:110:MET:H    | 1.65                     | 0.45              |
| 37:BP:38:ARG:CZ    | 37:BP:39:LEU:H     | 2.29                     | 0.45              |
| 38:BQ:16:ILE:HD11  | 38:BQ:31:TYR:CD1   | 2.52                     | 0.45              |
| 38:BQ:35:PHE:CA    | 38:BQ:39:ILE:HD12  | 2.46                     | 0.45              |
| 46:BZ:49:ARG:C     | 46:BZ:51:VAL:N     | 2.72                     | 0.45              |
| 47:B0:35:GLU:HG2   | 47:B0:36:LYS:N     | 2.30                     | 0.45              |
| 50:B3:44:ARG:NH1   | 50:B3:44:ARG:HG2   | 2.32                     | 0.45              |
| 52:BI:14:ALA:CB    | 52:BI:50:LYS:HA    | 2.47                     | 0.45              |
| 52:BI:62:ALA:C     | 52:BI:64:ARG:N     | 2.75                     | 0.45              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:224:U:H2'    | 1:CA:225:C:H6      | 1.82                     | 0.45              |
| 1:CA:295:C:H2'    | 1:CA:296:U:C6      | 2.52                     | 0.45              |
| 1:CA:343:U:H2'    | 1:CA:345:C:C5      | 2.52                     | 0.45              |
| 1:CA:432:A:C2'    | 1:CA:433:G:H5'     | 2.47                     | 0.45              |
| 1:CA:478:A:H2'    | 1:CA:479:U:O4'     | 2.15                     | 0.45              |
| 1:CA:957:U:H2'    | 1:CA:959:A:OP2     | 2.17                     | 0.45              |
| 1:CA:1250:A:C5'   | 8:CI:69:GLY:H      | 2.29                     | 0.45              |
| 1:CA:1319:A:H2'   | 1:CA:1323:G:N7     | 2.32                     | 0.45              |
| 2:CC:53:ARG:HA    | 2:CC:113:LYS:CE    | 2.47                     | 0.45              |
| 2:CC:63:ILE:HG12  | 2:CC:65:VAL:CG2    | 2.46                     | 0.45              |
| 3:CD:98:ASP:OD2   | 3:CD:99:ASN:N      | 2.50                     | 0.45              |
| 3:CD:104:MET:HG3  | 3:CD:142:VAL:HG21  | 1.99                     | 0.45              |
| 4:CE:14:LEU:HD22  | 4:CE:15:ILE:N      | 2.32                     | 0.45              |
| 4:CE:137:ARG:NH1  | 4:CE:137:ARG:HG2   | 2.31                     | 0.45              |
| 7:CH:12:ARG:HD2   | 7:CH:26:MET:HE2    | 1.99                     | 0.45              |
| 8:CI:88:GLU:HA    | 8:CI:91:GLU:OE2    | 2.16                     | 0.45              |
| 8:CI:115:VAL:HG22 | 8:CI:116:GLY:N     | 2.32                     | 0.45              |
| 11:CL:41:PRO:HG2  | 11:CL:45:ASN:O     | 2.16                     | 0.45              |
| 17:CR:33:THR:HG23 | 17:CR:35:SER:H     | 1.81                     | 0.45              |
| 18:CS:50:VAL:CG2  | 18:CS:70:LEU:HG    | 2.45                     | 0.45              |
| 21:CU:7:GLU:OE1   | 21:CU:11:PHE:HZ    | 2.00                     | 0.45              |
| 22:DA:55:U:O2'    | 28:DF:25:MET:HB3   | 2.16                     | 0.45              |
| 23:DB:154:U:H2'   | 23:DB:155:A:C8     | 2.52                     | 0.45              |
| 23:DB:303:G:H2'   | 23:DB:304:U:H6     | 1.82                     | 0.45              |
| 23:DB:438:G:O2'   | 23:DB:439:A:H5'    | 2.16                     | 0.45              |
| 23:DB:1148:U:O2'  | 23:DB:1149:G:H5'   | 2.15                     | 0.45              |
| 23:DB:1221:C:H2'  | 23:DB:1222:U:H6    | 1.82                     | 0.45              |
| 23:DB:1251:C:H5'' | 38:DQ:5:ARG:NH1    | 2.32                     | 0.45              |
| 23:DB:1454:C:H5'  | 35:DN:63:ARG:HD2   | 1.97                     | 0.45              |
| 23:DB:1880:U:H2'  | 23:DB:1881:C:C6    | 2.52                     | 0.45              |
| 23:DB:2065:C:H2'  | 23:DB:2066:C:C6    | 2.51                     | 0.45              |
| 23:DB:2460:U:H2'  | 23:DB:2461:A:H8    | 1.81                     | 0.45              |
| 23:DB:2649:C:H2'  | 23:DB:2650:U:C6    | 2.52                     | 0.45              |
| 23:DB:2712:C:H2'  | 23:DB:2714:G:O3'   | 2.17                     | 0.45              |
| 23:DB:2769:U:O2'  | 23:DB:2770:G:H5'   | 2.16                     | 0.45              |
| 25:DC:71:ASP:HA   | 25:DC:117:SER:OG   | 2.17                     | 0.45              |
| 26:DD:7:LYS:HB3   | 26:DD:201:LEU:HD22 | 1.98                     | 0.45              |
| 26:DD:14:ILE:O    | 26:DD:15:PHE:HD1   | 2.00                     | 0.45              |
| 26:DD:77:ARG:HB2  | 26:DD:77:ARG:CZ    | 2.47                     | 0.45              |
| 26:DD:172:VAL:CG1 | 26:DD:175:LEU:HD11 | 2.46                     | 0.45              |
| 27:DE:17:THR:CG2  | 27:DE:18:THR:H     | 2.28                     | 0.45              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 28:DF:15:LEU:HD13  | 28:DF:28:PRO:HG2  | 1.98                     | 0.45              |
| 29:DG:138:GLN:HE22 | 29:DG:142:GLN:HG3 | 1.82                     | 0.45              |
| 30:DH:4:ILE:HD13   | 30:DH:37:VAL:HG13 | 1.98                     | 0.45              |
| 30:DH:8:LYS:HA     | 30:DH:13:GLY:O    | 2.17                     | 0.45              |
| 30:DH:94:ILE:O     | 30:DH:122:LEU:HB2 | 2.16                     | 0.45              |
| 31:DJ:5:THR:HG23   | 31:DJ:7:LYS:HD3   | 1.99                     | 0.45              |
| 32:DK:78:ARG:H     | 37:DP:72:VAL:HG23 | 1.82                     | 0.45              |
| 33:DL:7:SER:CB     | 33:DL:8:PRO:CD    | 2.87                     | 0.45              |
| 33:DL:94:THR:OG1   | 33:DL:95:LEU:HD12 | 2.16                     | 0.45              |
| 34:DM:134:THR:HG22 | 34:DM:135:VAL:N   | 2.24                     | 0.45              |
| 36:DO:86:GLY:O     | 36:DO:88:LYS:N    | 2.50                     | 0.45              |
| 38:DQ:17:LEU:O     | 38:DQ:20:ALA:HB3  | 2.17                     | 0.45              |
| 39:DR:11:GLN:N     | 39:DR:21:ARG:NH2  | 2.64                     | 0.45              |
| 42:DU:85:ARG:O     | 42:DU:87:GLU:N    | 2.50                     | 0.45              |
| 45:DY:3:THR:O      | 45:DY:36:GLU:HA   | 2.16                     | 0.45              |
| 1:AA:385:C:O2'     | 1:AA:386:C:H5'    | 2.17                     | 0.45              |
| 1:AA:408:A:P       | 3:AD:109:THR:HG21 | 2.57                     | 0.45              |
| 1:AA:521:G:O2'     | 1:AA:522:C:H5'    | 2.17                     | 0.45              |
| 1:AA:551:U:O2'     | 1:AA:552:U:H5'    | 2.17                     | 0.45              |
| 1:AA:781:A:H2'     | 1:AA:782:A:C5'    | 2.38                     | 0.45              |
| 1:AA:957:U:H2'     | 1:AA:959:A:OP2    | 2.17                     | 0.45              |
| 1:AA:1148:U:H5'    | 8:AI:6:TYR:OH     | 2.17                     | 0.45              |
| 1:AA:1171:A:HO2'   | 1:AA:1172:C:H5'   | 1.82                     | 0.45              |
| 1:AA:1323:G:O2'    | 1:AA:1362:A:O4'   | 2.35                     | 0.45              |
| 1:AA:1478:U:H2'    | 1:AA:1479:C:C6    | 2.52                     | 0.45              |
| 1:AA:1481:U:H2'    | 1:AA:1482:G:C8    | 2.52                     | 0.45              |
| 1:AA:1521:C:O2'    | 1:AA:1522:U:H5'   | 2.17                     | 0.45              |
| 3:AD:94:GLU:HA     | 3:AD:94:GLU:OE2   | 2.16                     | 0.45              |
| 3:AD:145:ARG:HH11  | 3:AD:145:ARG:CB   | 2.29                     | 0.45              |
| 4:AE:56:PRO:O      | 4:AE:59:ILE:HG22  | 2.16                     | 0.45              |
| 4:AE:88:HIS:CE1    | 4:AE:89:THR:HG1   | 2.34                     | 0.45              |
| 6:AG:73:GLU:OE2    | 6:AG:90:VAL:HG12  | 2.17                     | 0.45              |
| 12:AM:52:ILE:HG23  | 12:AM:53:ASP:N    | 2.32                     | 0.45              |
| 13:AN:32:ASP:C     | 13:AN:40:ARG:HE   | 2.25                     | 0.45              |
| 14:AO:77:TYR:O     | 14:AO:81:ILE:HG23 | 2.17                     | 0.45              |
| 16:AQ:29:LYS:HD3   | 16:AQ:35:LYS:CA   | 2.47                     | 0.45              |
| 17:AR:22:TYR:CD2   | 17:AR:60:ARG:HD2  | 2.51                     | 0.45              |
| 18:AS:64:GLU:O     | 18:AS:66:VAL:HG23 | 2.17                     | 0.45              |
| 20:AB:81:ASP:O     | 20:AB:85:SER:HB2  | 2.17                     | 0.45              |
| 23:BB:493:G:H2'    | 23:BB:494:G:O4'   | 2.17                     | 0.45              |
| 23:BB:640:C:H1'    | 50:B3:44:ARG:NH2  | 2.32                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:952:G:C6     | 23:BB:966:G:C6     | 3.05                     | 0.45              |
| 23:BB:1064:C:C4'   | 52:BI:90:GLY:HA2   | 2.47                     | 0.45              |
| 23:BB:1487:U:H2'   | 23:BB:1488:C:C6    | 2.50                     | 0.45              |
| 23:BB:1736:U:H2'   | 23:BB:1737:G:C8    | 2.52                     | 0.45              |
| 23:BB:1985:C:O2'   | 23:BB:1986:C:H5'   | 2.17                     | 0.45              |
| 23:BB:2065:C:H2'   | 23:BB:2066:C:C6    | 2.51                     | 0.45              |
| 23:BB:2671:G:H2'   | 23:BB:2672:U:H6    | 1.80                     | 0.45              |
| 26:BD:128:ARG:CA   | 26:BD:128:ARG:NE   | 2.80                     | 0.45              |
| 28:BF:13:LYS:HD3   | 28:BF:16:MET:HG3   | 1.99                     | 0.45              |
| 28:BF:132:ARG:NH2  | 28:BF:147:ARG:HE   | 2.15                     | 0.45              |
| 30:BH:55:GLU:C     | 30:BH:57:LYS:H     | 2.23                     | 0.45              |
| 32:BK:20:MET:O     | 32:BK:42:THR:N     | 2.49                     | 0.45              |
| 33:BL:77:ILE:HD12  | 33:BL:110:VAL:HG22 | 1.99                     | 0.45              |
| 34:BM:31:PHE:HA    | 34:BM:128:THR:HG22 | 1.97                     | 0.45              |
| 35:BN:38:LEU:N     | 35:BN:39:PRO:CD    | 2.80                     | 0.45              |
| 36:BO:106:LEU:HD13 | 36:BO:106:LEU:C    | 2.42                     | 0.45              |
| 37:BP:9:GLN:HB3    | 37:BP:56:SER:HB2   | 1.97                     | 0.45              |
| 37:BP:26:GLU:O     | 37:BP:46:VAL:HG22  | 2.17                     | 0.45              |
| 38:BQ:16:ILE:HD11  | 38:BQ:31:TYR:HD1   | 1.82                     | 0.45              |
| 38:BQ:19:GLN:NE2   | 38:BQ:38:VAL:HG23  | 2.32                     | 0.45              |
| 38:BQ:92:LYS:CD    | 38:BQ:93:ILE:N     | 2.80                     | 0.45              |
| 40:BS:70:LYS:O     | 40:BS:71:VAL:HB    | 2.17                     | 0.45              |
| 42:BU:2:ALA:O      | 42:BU:3:LYS:HD3    | 2.16                     | 0.45              |
| 48:B1:7:LYS:HD2    | 48:B1:7:LYS:C      | 2.42                     | 0.45              |
| 48:B1:20:TYR:O     | 48:B1:21:THR:HB    | 2.17                     | 0.45              |
| 48:B1:40:PRO:HA    | 48:B1:48:TYR:OH    | 2.16                     | 0.45              |
| 50:B3:29:ARG:HA    | 50:B3:33:THR:HG21  | 1.95                     | 0.45              |
| 51:B4:7:VAL:HB     | 51:B4:35:GLN:NE2   | 2.31                     | 0.45              |
| 51:B4:24:ARG:HH22  | 51:B4:36:ARG:HD3   | 1.79                     | 0.45              |
| 1:CA:24:U:O2'      | 1:CA:25:C:H5'      | 2.16                     | 0.45              |
| 1:CA:182:A:O2'     | 1:CA:183:C:O5'     | 2.34                     | 0.45              |
| 1:CA:285:C:H2'     | 1:CA:286:C:H6      | 1.81                     | 0.45              |
| 1:CA:817:C:C2      | 1:CA:819:A:O4'     | 2.70                     | 0.45              |
| 1:CA:953:G:H3'     | 1:CA:954:G:H8      | 1.82                     | 0.45              |
| 1:CA:1147:C:HO2'   | 8:CI:6:TYR:HE2     | 1.64                     | 0.45              |
| 2:CC:129:PHE:CG    | 2:CC:130:ARG:N     | 2.85                     | 0.45              |
| 6:CG:29:LEU:HG     | 6:CG:104:VAL:HG22  | 1.99                     | 0.45              |
| 11:CL:89:LEU:HD22  | 11:CL:89:LEU:N     | 2.32                     | 0.45              |
| 11:CL:91:GLY:O     | 11:CL:93:ARG:NE    | 2.50                     | 0.45              |
| 12:CM:73:SER:O     | 12:CM:77:LYS:HG3   | 2.17                     | 0.45              |
| 15:CP:57:ILE:HD11  | 15:CP:75:ILE:HD11  | 1.98                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:13:G:H2'    | 22:DA:14:U:H5''   | 1.99                     | 0.45              |
| 23:DB:631:A:O2'   | 33:DL:66:PHE:CD1  | 2.70                     | 0.45              |
| 23:DB:743:A:OP1   | 26:DD:134:HIS:CD2 | 2.70                     | 0.45              |
| 23:DB:743:A:OP1   | 26:DD:134:HIS:NE2 | 2.50                     | 0.45              |
| 23:DB:1131:G:N7   | 23:DB:2025:C:H4'  | 2.32                     | 0.45              |
| 23:DB:1190:G:OP1  | 33:DL:38:GLN:CB   | 2.65                     | 0.45              |
| 23:DB:1205:A:N7   | 27:DE:164:LEU:CD1 | 2.80                     | 0.45              |
| 23:DB:1509:A:C5'  | 23:DB:1510:G:H5'  | 2.47                     | 0.45              |
| 23:DB:1585:C:H2'  | 23:DB:1586:A:C8   | 2.52                     | 0.45              |
| 23:DB:1712:U:H3'  | 23:DB:1713:A:C5'  | 2.46                     | 0.45              |
| 23:DB:2420:C:OP2  | 50:D3:31:ILE:HA   | 2.17                     | 0.45              |
| 23:DB:2637:U:O2'  | 23:DB:2638:G:H5'  | 2.17                     | 0.45              |
| 23:DB:2733:A:H2'  | 23:DB:2734:A:O4'  | 2.17                     | 0.45              |
| 26:DD:40:LEU:O    | 26:DD:41:ALA:HB3  | 2.17                     | 0.45              |
| 28:DF:16:MET:HE2  | 28:DF:16:MET:HA   | 1.99                     | 0.45              |
| 30:DH:4:ILE:O     | 30:DH:5:LEU:HD22  | 2.17                     | 0.45              |
| 30:DH:7:ASP:HB3   | 30:DH:8:LYS:H     | 1.60                     | 0.45              |
| 31:DJ:58:ASN:O    | 31:DJ:60:ASP:N    | 2.45                     | 0.45              |
| 31:DJ:94:ALA:HB3  | 31:DJ:95:ARG:HE   | 1.82                     | 0.45              |
| 35:DN:45:ARG:NH2  | 35:DN:97:ILE:HG12 | 2.31                     | 0.45              |
| 39:DR:37:GLU:CG   | 39:DR:62:GLU:HG3  | 2.45                     | 0.45              |
| 41:DT:15:HIS:HB3  | 41:DT:31:VAL:CG1  | 2.47                     | 0.45              |
| 41:DT:85:VAL:HG23 | 41:DT:86:THR:N    | 2.32                     | 0.45              |
| 47:D0:29:VAL:HG23 | 47:D0:32:THR:OG1  | 2.16                     | 0.45              |
| 48:D1:14:ALA:CB   | 48:D1:19:PHE:HB3  | 2.47                     | 0.45              |
| 48:D1:40:PRO:HD2  | 48:D1:44:GLN:C    | 2.42                     | 0.45              |
| 1:AA:432:A:C2'    | 1:AA:433:G:H5'    | 2.47                     | 0.44              |
| 1:AA:649:A:H2'    | 1:AA:650:G:O4'    | 2.17                     | 0.44              |
| 1:AA:817:C:C2     | 1:AA:819:A:O4'    | 2.70                     | 0.44              |
| 1:AA:1282:C:H2'   | 1:AA:1283:U:C6    | 2.52                     | 0.44              |
| 1:AA:1439:G:H2'   | 1:AA:1440:U:O4'   | 2.18                     | 0.44              |
| 2:AC:25:THR:CG2   | 13:AN:74:ARG:HD2  | 2.47                     | 0.44              |
| 2:AC:113:LYS:HZ3  | 2:AC:117:ASP:CG   | 2.24                     | 0.44              |
| 3:AD:10:LEU:HD21  | 3:AD:62:ARG:CG    | 2.46                     | 0.44              |
| 5:AF:40:GLU:CG    | 5:AF:42:TRP:HE1   | 2.27                     | 0.44              |
| 13:AN:50:LEU:CG   | 13:AN:51:PRO:HD3  | 2.46                     | 0.44              |
| 14:AO:22:GLY:O    | 14:AO:23:SER:C    | 2.60                     | 0.44              |
| 14:AO:70:LYS:HG2  | 14:AO:77:TYR:CG   | 2.52                     | 0.44              |
| 15:AP:39:PHE:HE2  | 15:AP:70:ARG:NH2  | 2.15                     | 0.44              |
| 17:AR:64:LEU:CB   | 17:AR:66:LEU:HG   | 2.47                     | 0.44              |
| 18:AS:50:VAL:H    | 18:AS:57:VAL:H    | 1.64                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:AU:17:ARG:CA    | 21:AU:20:ARG:HB3   | 2.43                     | 0.44              |
| 23:BB:126:A:OP2    | 49:B2:45:SER:OG    | 2.29                     | 0.44              |
| 23:BB:138:U:H2'    | 23:BB:140:C:Cl'    | 2.45                     | 0.44              |
| 23:BB:699:A:H2'    | 23:BB:700:G:O4'    | 2.17                     | 0.44              |
| 23:BB:807:U:H2'    | 23:BB:808:G:H8     | 1.81                     | 0.44              |
| 23:BB:844:A:H2     | 23:BB:845:A:N1     | 2.16                     | 0.44              |
| 23:BB:1292:G:H2'   | 23:BB:1293:C:H6    | 1.82                     | 0.44              |
| 23:BB:1773:A:C8    | 23:BB:1829:A:C8    | 3.05                     | 0.44              |
| 23:BB:1790:C:H4'   | 25:BC:207:ALA:CB   | 2.46                     | 0.44              |
| 23:BB:1880:U:H2'   | 23:BB:1881:C:C6    | 2.52                     | 0.44              |
| 23:BB:2285:C:OP1   | 48:B1:26:LYS:HE3   | 2.17                     | 0.44              |
| 23:BB:2304:G:N2    | 23:BB:2312:U:H3    | 2.15                     | 0.44              |
| 23:BB:2373:G:H2'   | 23:BB:2374:C:H6    | 1.80                     | 0.44              |
| 23:BB:2464:G:H2'   | 23:BB:2465:C:C6    | 2.51                     | 0.44              |
| 23:BB:2576:G:P     | 26:BD:149:ASN:CB   | 2.94                     | 0.44              |
| 23:BB:2774:C:P     | 26:BD:169:ARG:HG3  | 2.57                     | 0.44              |
| 25:BC:90:ILE:CG2   | 25:BC:91:ALA:N     | 2.79                     | 0.44              |
| 25:BC:224:MET:HE3  | 25:BC:232:GLY:HA2  | 1.98                     | 0.44              |
| 28:BF:101:ARG:HD2  | 28:BF:105:ILE:HD12 | 1.99                     | 0.44              |
| 29:BG:158:GLY:CA   | 29:BG:170:THR:HG21 | 2.46                     | 0.44              |
| 30:BH:35:LYS:HD2   | 30:BH:35:LYS:H     | 1.82                     | 0.44              |
| 30:BH:147:VAL:HG12 | 30:BH:148:ALA:N    | 2.32                     | 0.44              |
| 32:BK:24:VAL:HG12  | 32:BK:30:ARG:HB3   | 1.98                     | 0.44              |
| 35:BN:86:ARG:HH21  | 35:BN:116:VAL:HG11 | 1.82                     | 0.44              |
| 37:BP:31:VAL:HA    | 37:BP:81:ASP:CB    | 2.48                     | 0.44              |
| 38:BQ:16:ILE:HD12  | 38:BQ:16:ILE:C     | 2.42                     | 0.44              |
| 38:BQ:19:GLN:O     | 38:BQ:20:ALA:C     | 2.59                     | 0.44              |
| 44:BX:36:GLN:CD    | 44:BX:37:LEU:HG    | 2.42                     | 0.44              |
| 46:BZ:31:ASP:HA    | 46:BZ:47:LYS:O     | 2.17                     | 0.44              |
| 47:B0:51:ARG:O     | 47:B0:52:LYS:HD2   | 2.18                     | 0.44              |
| 52:BI:135:MET:HE2  | 52:BI:137:LEU:CD1  | 2.47                     | 0.44              |
| 1:CA:385:C:O2'     | 1:CA:386:C:H5'     | 2.17                     | 0.44              |
| 1:CA:1371:G:O3'    | 8:CI:70:GLY:HA3    | 2.17                     | 0.44              |
| 1:CA:1426:G:H2'    | 1:CA:1427:C:C6     | 2.52                     | 0.44              |
| 1:CA:1526:G:OP1    | 21:CU:37:TYR:HB3   | 2.17                     | 0.44              |
| 3:CD:18:LEU:N      | 3:CD:18:LEU:HD22   | 2.31                     | 0.44              |
| 3:CD:71:PHE:CE2    | 3:CD:89:LEU:HD11   | 2.51                     | 0.44              |
| 3:CD:74:TYR:HB3    | 3:CD:89:LEU:HD12   | 1.98                     | 0.44              |
| 3:CD:123:MET:CB    | 3:CD:128:VAL:HA    | 2.46                     | 0.44              |
| 3:CD:123:MET:HB3   | 3:CD:128:VAL:HA    | 1.99                     | 0.44              |
| 3:CD:172:VAL:HG22  | 3:CD:173:ASP:N     | 2.32                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:CF:94:HIS:O     | 5:CF:95:ALA:C      | 2.59                     | 0.44              |
| 9:CJ:19:ASP:HA    | 9:CJ:22:THR:HG22   | 1.99                     | 0.44              |
| 10:CK:70:ALA:CA   | 10:CK:73:VAL:HG22  | 2.47                     | 0.44              |
| 10:CK:100:ASN:C   | 10:CK:102:ALA:H    | 2.25                     | 0.44              |
| 12:CM:84:CYS:O    | 12:CM:88:LEU:HG    | 2.16                     | 0.44              |
| 13:CN:24:ALA:C    | 13:CN:26:LEU:H     | 2.25                     | 0.44              |
| 22:DA:107:G:O2'   | 22:DA:108:A:H5'    | 2.17                     | 0.44              |
| 23:DB:231:A:H3'   | 23:DB:232:G:C8     | 2.52                     | 0.44              |
| 23:DB:1005:C:O2'  | 23:DB:1006:C:H5'   | 2.15                     | 0.44              |
| 23:DB:1021:A:N6   | 23:DB:1142:A:N6    | 2.54                     | 0.44              |
| 23:DB:1025:G:OP1  | 23:DB:1025:G:H8    | 2.00                     | 0.44              |
| 23:DB:1116:G:O2'  | 23:DB:1117:C:H5'   | 2.17                     | 0.44              |
| 23:DB:1180:U:H2'  | 23:DB:1181:U:O4'   | 2.17                     | 0.44              |
| 23:DB:1199:U:O2'  | 38:DQ:2:ARG:HB3    | 2.16                     | 0.44              |
| 23:DB:1914:C:H3'  | 23:DB:1914:C:OP2   | 2.18                     | 0.44              |
| 23:DB:2457:U:O2'  | 23:DB:2458:G:H5'   | 2.17                     | 0.44              |
| 23:DB:2598:A:P    | 25:DC:237:ARG:HH12 | 2.39                     | 0.44              |
| 25:DC:72:GLY:C    | 25:DC:73:ILE:HG13  | 2.42                     | 0.44              |
| 26:DD:31:ALA:HB3  | 26:DD:95:SER:HB2   | 1.99                     | 0.44              |
| 26:DD:45:TYR:HB3  | 26:DD:46:ARG:H     | 1.65                     | 0.44              |
| 28:DF:121:PHE:CE1 | 28:DF:166:ARG:HG2  | 2.52                     | 0.44              |
| 30:DH:19:VAL:HG22 | 30:DH:20:ASN:N     | 2.32                     | 0.44              |
| 31:DJ:73:VAL:HG22 | 31:DJ:74:TYR:H     | 1.80                     | 0.44              |
| 38:DQ:52:ARG:HG2  | 38:DQ:53:LYS:H     | 1.83                     | 0.44              |
| 45:DY:17:PRO:HD2  | 45:DY:18:LYS:NZ    | 2.31                     | 0.44              |
| 50:D3:21:PHE:O    | 50:D3:48:MET:HB2   | 2.16                     | 0.44              |
| 51:D4:9:LYS:O     | 51:D4:25:VAL:HA    | 2.18                     | 0.44              |
| 1:AA:178:C:O2'    | 1:AA:179:A:H5'     | 2.17                     | 0.44              |
| 1:AA:343:U:H2'    | 1:AA:345:C:C5      | 2.52                     | 0.44              |
| 1:AA:668:G:O2'    | 1:AA:669:G:H5'     | 2.17                     | 0.44              |
| 1:AA:734:G:H2'    | 1:AA:735:C:C6      | 2.53                     | 0.44              |
| 1:AA:1262:C:H2'   | 1:AA:1263:C:O4'    | 2.17                     | 0.44              |
| 4:AE:16:ALA:O     | 4:AE:34:ALA:HA     | 2.16                     | 0.44              |
| 6:AG:74:VAL:HG12  | 6:AG:75:LYS:N      | 2.30                     | 0.44              |
| 6:AG:87:PRO:CG    | 6:AG:151:ALA:HB2   | 2.46                     | 0.44              |
| 7:AH:93:LYS:HZ2   | 7:AH:93:LYS:H      | 1.64                     | 0.44              |
| 11:AL:32:VAL:O    | 11:AL:33:CYS:HB2   | 2.15                     | 0.44              |
| 13:AN:60:ARG:NE   | 13:AN:62:ARG:HE    | 2.15                     | 0.44              |
| 15:AP:39:PHE:CE1  | 15:AP:74:LEU:HD22  | 2.52                     | 0.44              |
| 15:AP:40:ASN:HB3  | 15:AP:49:GLY:O     | 2.17                     | 0.44              |
| 16:AQ:44:HIS:O    | 16:AQ:72:TRP:HB2   | 2.16                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BB:173:A:H2'   | 23:BB:174:U:C6    | 2.52                     | 0.44              |
| 23:BB:269:C:O2'   | 23:BB:270:A:H5'   | 2.17                     | 0.44              |
| 23:BB:273:G:H2'   | 23:BB:274:C:C6    | 2.53                     | 0.44              |
| 23:BB:689:A:H2'   | 23:BB:690:G:C8    | 2.52                     | 0.44              |
| 23:BB:701:G:O2'   | 23:BB:702:U:H5'   | 2.16                     | 0.44              |
| 23:BB:718:A:H2'   | 23:BB:719:C:H5'   | 1.99                     | 0.44              |
| 23:BB:1157:G:H1'  | 45:BY:10:ARG:NH2  | 2.31                     | 0.44              |
| 23:BB:1263:U:H4'  | 47:B0:8:THR:HB    | 2.00                     | 0.44              |
| 23:BB:1286:A:H1'  | 23:BB:1288:G:OP2  | 2.17                     | 0.44              |
| 23:BB:1541:C:O2'  | 23:BB:1542:U:H5'  | 2.17                     | 0.44              |
| 23:BB:1589:U:H2'  | 23:BB:1590:A:C8   | 2.52                     | 0.44              |
| 23:BB:2065:C:C2   | 23:BB:2066:C:C5   | 3.05                     | 0.44              |
| 23:BB:2204:G:O2'  | 23:BB:2205:A:H5'  | 2.17                     | 0.44              |
| 23:BB:2220:U:O2'  | 23:BB:2221:G:H5'  | 2.17                     | 0.44              |
| 23:BB:2257:U:OP1  | 43:BW:5:ALA:HB2   | 2.18                     | 0.44              |
| 23:BB:2306:C:N4   | 28:BF:38:GLY:H    | 2.03                     | 0.44              |
| 23:BB:2354:C:H4'  | 43:BW:30:VAL:HG13 | 1.98                     | 0.44              |
| 23:BB:2466:C:O2'  | 23:BB:2467:C:H5'  | 2.17                     | 0.44              |
| 23:BB:2521:C:O2'  | 23:BB:2522:U:H5'  | 2.17                     | 0.44              |
| 23:BB:2678:C:O2'  | 23:BB:2679:A:H5'  | 2.17                     | 0.44              |
| 25:BC:27:LYS:HA   | 25:BC:79:ARG:CZ   | 2.48                     | 0.44              |
| 25:BC:115:ILE:HA  | 25:BC:126:GLY:CA  | 2.47                     | 0.44              |
| 25:BC:245:THR:O   | 25:BC:246:PRO:C   | 2.61                     | 0.44              |
| 26:BD:151:THR:HB  | 26:BD:152:PRO:CD  | 2.48                     | 0.44              |
| 29:BG:154:GLU:OE2 | 29:BG:159:LYS:HG2 | 2.17                     | 0.44              |
| 30:BH:57:LYS:HE3  | 30:BH:57:LYS:N    | 2.32                     | 0.44              |
| 32:BK:121:GLU:HG2 | 37:BP:67:GLU:OE2  | 2.16                     | 0.44              |
| 33:BL:58:TYR:O    | 33:BL:61:LEU:HD21 | 2.17                     | 0.44              |
| 36:BO:8:ILE:O     | 36:BO:10:ARG:N    | 2.50                     | 0.44              |
| 39:BR:35:PHE:HB2  | 39:BR:64:VAL:HG21 | 1.98                     | 0.44              |
| 39:BR:47:VAL:C    | 39:BR:49:ILE:N    | 2.75                     | 0.44              |
| 43:BW:39:GLN:HA   | 43:BW:68:PHE:HA   | 1.98                     | 0.44              |
| 52:BI:52:LEU:HD12 | 52:BI:52:LEU:N    | 2.32                     | 0.44              |
| 1:CA:428:G:H4'    | 1:CA:429:U:O5'    | 2.17                     | 0.44              |
| 1:CA:676:A:H5''   | 10:CK:114:PRO:CB  | 2.47                     | 0.44              |
| 1:CA:836:G:H2'    | 1:CA:837:U:C6     | 2.52                     | 0.44              |
| 1:CA:857:C:H2'    | 1:CA:858:G:O4'    | 2.17                     | 0.44              |
| 1:CA:983:A:O2'    | 1:CA:1049:U:O2'   | 2.32                     | 0.44              |
| 1:CA:1030:U:HO2'  | 1:CA:1031:C:P     | 2.38                     | 0.44              |
| 1:CA:1031:C:H5'   | 1:CA:1032:G:C4    | 2.53                     | 0.44              |
| 2:CC:129:PHE:CZ   | 2:CC:156:LEU:HD13 | 2.52                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:CE:10:LEU:HA    | 4:CE:39:GLY:O      | 2.17                     | 0.44              |
| 4:CE:37:VAL:HG12  | 4:CE:116:VAL:HG21  | 1.99                     | 0.44              |
| 4:CE:109:ALA:HB3  | 4:CE:135:VAL:HG11  | 1.99                     | 0.44              |
| 7:CH:72:GLU:HB3   | 7:CH:129:ALA:HB2   | 1.98                     | 0.44              |
| 7:CH:76:ARG:NE    | 7:CH:125:ILE:HG23  | 2.32                     | 0.44              |
| 8:CI:38:PHE:HB2   | 8:CI:44:ARG:HG3    | 2.00                     | 0.44              |
| 9:CJ:17:LEU:HD11  | 9:CJ:96:VAL:HG12   | 1.98                     | 0.44              |
| 9:CJ:98:VAL:HG23  | 9:CJ:98:VAL:O      | 2.18                     | 0.44              |
| 14:CO:23:SER:HB3  | 14:CO:26:VAL:HG23  | 1.99                     | 0.44              |
| 16:CQ:18:LYS:HA   | 16:CQ:47:ASP:O     | 2.17                     | 0.44              |
| 21:CU:25:ALA:C    | 21:CU:27:VAL:N     | 2.75                     | 0.44              |
| 22:DA:14:U:H4'    | 22:DA:70:C:O2      | 2.17                     | 0.44              |
| 23:DB:152:A:H2'   | 23:DB:153:U:C6     | 2.53                     | 0.44              |
| 23:DB:689:A:H2'   | 23:DB:690:G:C8     | 2.52                     | 0.44              |
| 23:DB:709:U:H2'   | 23:DB:710:U:H6     | 1.81                     | 0.44              |
| 23:DB:727:A:OP1   | 23:DB:1431:A:O2'   | 2.35                     | 0.44              |
| 23:DB:807:U:H2'   | 23:DB:808:G:H8     | 1.81                     | 0.44              |
| 23:DB:822:G:H2'   | 23:DB:823:C:C6     | 2.53                     | 0.44              |
| 23:DB:1563:U:O2'  | 23:DB:1564:C:H5'   | 2.17                     | 0.44              |
| 23:DB:1724:G:H2'  | 23:DB:1725:U:H6    | 1.82                     | 0.44              |
| 23:DB:2038:G:H2'  | 23:DB:2039:U:H6    | 1.82                     | 0.44              |
| 23:DB:2415:G:H4'  | 33:DL:66:PHE:HB2   | 2.00                     | 0.44              |
| 25:DC:24:HIS:HB3  | 25:DC:25:LYS:H     | 1.54                     | 0.44              |
| 25:DC:137:GLY:O   | 25:DC:140:VAL:HG13 | 2.16                     | 0.44              |
| 25:DC:155:ARG:HG2 | 25:DC:155:ARG:NH2  | 2.31                     | 0.44              |
| 27:DE:109:LEU:HA  | 27:DE:117:ARG:NH1  | 2.32                     | 0.44              |
| 29:DG:98:LYS:HB3  | 29:DG:101:VAL:HG23 | 1.98                     | 0.44              |
| 30:DH:35:LYS:NZ   | 30:DH:37:VAL:HG23  | 2.32                     | 0.44              |
| 31:DJ:133:ALA:C   | 31:DJ:135:GLN:H    | 2.23                     | 0.44              |
| 33:DL:58:TYR:HA   | 33:DL:62:PRO:CG    | 2.47                     | 0.44              |
| 34:DM:96:ILE:H    | 34:DM:98:PRO:HD3   | 1.83                     | 0.44              |
| 39:DR:73:LYS:N    | 39:DR:73:LYS:HD2   | 2.32                     | 0.44              |
| 45:DY:8:GLN:HE21  | 45:DY:23:LEU:HD12  | 1.82                     | 0.44              |
| 46:DZ:48:GLN:O    | 46:DZ:51:VAL:HB    | 2.17                     | 0.44              |
| 48:D1:42:VAL:HG12 | 48:D1:43:ARG:HG2   | 1.99                     | 0.44              |
| 52:DI:63:ASP:C    | 52:DI:65:SER:H     | 2.24                     | 0.44              |
| 1:AA:28:A:H2'     | 1:AA:29:U:O4'      | 2.17                     | 0.44              |
| 1:AA:541:G:H2'    | 1:AA:542:G:C8      | 2.52                     | 0.44              |
| 1:AA:1085:U:H3'   | 1:AA:1086:U:C5     | 2.53                     | 0.44              |
| 1:AA:1190:G:OP1   | 2:AC:4:VAL:HG12    | 2.17                     | 0.44              |
| 2:AC:70:ALA:CB    | 2:AC:108:PRO:HB3   | 2.47                     | 0.44              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:AI:51:LEU:CD1   | 8:AI:82:ILE:HG21   | 2.47                     | 0.44              |
| 8:AI:118:ARG:HH22 | 8:AI:122:ARG:HH21  | 1.66                     | 0.44              |
| 13:AN:73:LEU:HD12 | 13:AN:73:LEU:N     | 2.32                     | 0.44              |
| 15:AP:1:MET:H3    | 15:AP:24:SER:HB3   | 1.81                     | 0.44              |
| 15:AP:12:LYS:C    | 15:AP:14:ARG:H     | 2.24                     | 0.44              |
| 17:AR:21:ASP:CG   | 17:AR:22:TYR:N     | 2.76                     | 0.44              |
| 20:AB:172:ILE:O   | 20:AB:175:ALA:HB3  | 2.17                     | 0.44              |
| 20:AB:175:ALA:C   | 20:AB:177:ASN:H    | 2.24                     | 0.44              |
| 23:BB:39:G:H2'    | 23:BB:40:U:C6      | 2.52                     | 0.44              |
| 23:BB:185:G:H2'   | 23:BB:186:G:O4'    | 2.17                     | 0.44              |
| 23:BB:320:A:OP2   | 27:BE:132:LYS:HE2  | 2.18                     | 0.44              |
| 23:BB:376:G:H2'   | 23:BB:377:G:H8     | 1.81                     | 0.44              |
| 23:BB:435:C:C2'   | 23:BB:436:C:H5'    | 2.47                     | 0.44              |
| 23:BB:453:A:H4'   | 23:BB:472:A:N6     | 2.32                     | 0.44              |
| 23:BB:608:A:H2'   | 23:BB:609:A:H8     | 1.81                     | 0.44              |
| 23:BB:635:C:H3'   | 33:BL:109:LYS:NZ   | 2.33                     | 0.44              |
| 23:BB:728:G:H5'   | 25:BC:12:ARG:HH22  | 1.82                     | 0.44              |
| 23:BB:1560:G:C4   | 23:BB:1561:C:C5    | 3.06                     | 0.44              |
| 23:BB:1668:A:N3   | 23:BB:1670:C:C4    | 2.85                     | 0.44              |
| 23:BB:1678:A:O2'  | 23:BB:1679:A:H5'   | 2.16                     | 0.44              |
| 23:BB:1710:G:H2'  | 23:BB:1711:A:C8    | 2.52                     | 0.44              |
| 23:BB:1802:A:O3'  | 25:BC:255:LYS:HE2  | 2.18                     | 0.44              |
| 23:BB:2100:G:H3'  | 23:BB:2101:A:H8    | 1.82                     | 0.44              |
| 23:BB:2249:U:C4'  | 23:BB:2275:C:H5    | 2.29                     | 0.44              |
| 24:BV:79:ARG:HB3  | 24:BV:79:ARG:NH1   | 2.32                     | 0.44              |
| 25:BC:7:PRO:HB3   | 25:BC:25:LYS:HD3   | 1.98                     | 0.44              |
| 25:BC:243:PRO:HB3 | 25:BC:249:VAL:HG23 | 1.99                     | 0.44              |
| 26:BD:62:LYS:H    | 26:BD:62:LYS:CE    | 2.30                     | 0.44              |
| 27:BE:43:THR:O    | 27:BE:44:ARG:C     | 2.60                     | 0.44              |
| 29:BG:40:VAL:HG13 | 29:BG:52:GLY:O     | 2.18                     | 0.44              |
| 31:BJ:119:PHE:O   | 31:BJ:122:LEU:HG   | 2.18                     | 0.44              |
| 32:BK:25:LEU:C    | 32:BK:27:GLY:H     | 2.25                     | 0.44              |
| 36:BO:8:ILE:C     | 36:BO:10:ARG:N     | 2.76                     | 0.44              |
| 36:BO:10:ARG:HG3  | 36:BO:10:ARG:NH1   | 2.30                     | 0.44              |
| 36:BO:41:ALA:O    | 36:BO:42:PRO:C     | 2.60                     | 0.44              |
| 41:BT:47:VAL:HG12 | 41:BT:53:VAL:CG2   | 2.47                     | 0.44              |
| 41:BT:62:VAL:O    | 41:BT:63:VAL:CG1   | 2.61                     | 0.44              |
| 41:BT:87:LEU:HD22 | 41:BT:87:LEU:N     | 2.32                     | 0.44              |
| 42:BU:42:LYS:HD3  | 42:BU:60:LYS:CB    | 2.45                     | 0.44              |
| 43:BW:44:PHE:O    | 43:BW:76:ARG:N     | 2.50                     | 0.44              |
| 44:BX:15:ASN:O    | 44:BX:17:GLU:N     | 2.51                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 44:BX:19:LEU:C    | 44:BX:21:LEU:H   | 2.25                     | 0.44              |
| 45:BY:9:THR:HB    | 45:BY:54:VAL:CA  | 2.39                     | 0.44              |
| 45:BY:28:LEU:HA   | 45:BY:33:HIS:ND1 | 2.33                     | 0.44              |
| 47:B0:16:ARG:HD3  | 47:B0:16:ARG:C   | 2.42                     | 0.44              |
| 1:CA:28:A:H2'     | 1:CA:29:U:O4'    | 2.17                     | 0.44              |
| 1:CA:65:A:H2      | 1:CA:381:C:H2'   | 1.82                     | 0.44              |
| 1:CA:113:G:H2'    | 1:CA:114:U:H6    | 1.81                     | 0.44              |
| 1:CA:237:G:O2'    | 1:CA:238:A:H5'   | 2.18                     | 0.44              |
| 1:CA:238:A:C3'    | 1:CA:239:U:H5''  | 2.47                     | 0.44              |
| 1:CA:598:U:H2'    | 1:CA:599:C:H6    | 1.82                     | 0.44              |
| 1:CA:734:G:H2'    | 1:CA:735:C:C6    | 2.52                     | 0.44              |
| 1:CA:1456:A:H2'   | 1:CA:1457:G:C8   | 2.52                     | 0.44              |
| 3:CD:48:SER:O     | 3:CD:49:ASP:C    | 2.60                     | 0.44              |
| 4:CE:64:GLU:HA    | 4:CE:67:ARG:NH1  | 2.32                     | 0.44              |
| 4:CE:71:ILE:C     | 4:CE:72:ASN:HD22 | 2.24                     | 0.44              |
| 5:CF:68:GLN:HA    | 5:CF:71:ILE:CG2  | 2.45                     | 0.44              |
| 7:CH:75:GLN:HE21  | 7:CH:76:ARG:H    | 1.65                     | 0.44              |
| 8:CI:30:ASN:O     | 8:CI:31:GLN:HB2  | 2.17                     | 0.44              |
| 9:CJ:85:ASP:CG    | 9:CJ:89:ARG:HB2  | 2.43                     | 0.44              |
| 10:CK:16:SER:N    | 10:CK:78:ILE:HA  | 2.32                     | 0.44              |
| 12:CM:97:ARG:HH11 | 12:CM:97:ARG:HG2 | 1.82                     | 0.44              |
| 13:CN:63:CYS:CB   | 13:CN:68:ARG:H   | 2.25                     | 0.44              |
| 21:CU:43:GLU:O    | 21:CU:46:ARG:HB2 | 2.16                     | 0.44              |
| 23:DB:458:G:O2'   | 23:DB:459:U:C5   | 2.69                     | 0.44              |
| 23:DB:927:A:O2'   | 23:DB:928:A:H5'  | 2.18                     | 0.44              |
| 23:DB:974:G:H4'   | 39:DR:83:TYR:CZ  | 2.52                     | 0.44              |
| 23:DB:1064:C:H2'  | 23:DB:1065:U:O4' | 2.17                     | 0.44              |
| 23:DB:1266:G:OP2  | 47:D0:12:ARG:NH1 | 2.50                     | 0.44              |
| 23:DB:1317:G:H2'  | 23:DB:1318:U:O4' | 2.17                     | 0.44              |
| 23:DB:1359:A:H2'  | 23:DB:1360:G:O4' | 2.17                     | 0.44              |
| 23:DB:1541:C:O2'  | 23:DB:1542:U:H5' | 2.17                     | 0.44              |
| 23:DB:1560:G:C4   | 23:DB:1561:C:C5  | 3.06                     | 0.44              |
| 23:DB:1710:G:H2'  | 23:DB:1711:A:C8  | 2.52                     | 0.44              |
| 23:DB:1964:G:H4'  | 23:DB:1965:C:OP2 | 2.17                     | 0.44              |
| 23:DB:2259:U:O4'  | 23:DB:2427:C:H2' | 2.18                     | 0.44              |
| 23:DB:2270:A:H4'  | 43:DW:18:LYS:HB2 | 1.99                     | 0.44              |
| 23:DB:2491:U:H5'' | 23:DB:2570:G:H5' | 1.99                     | 0.44              |
| 24:DV:30:ILE:HB   | 24:DV:38:LEU:HB3 | 2.00                     | 0.44              |
| 25:DC:70:LYS:HD2  | 25:DC:95:TYR:CD1 | 2.52                     | 0.44              |
| 27:DE:48:THR:C    | 27:DE:49:ARG:HG2 | 2.41                     | 0.44              |
| 31:DJ:93:ILE:HG22 | 31:DJ:97:PRO:HA  | 1.99                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:DK:8:LEU:HD12  | 32:DK:8:LEU:H     | 1.82                     | 0.44              |
| 32:DK:17:ARG:HB2  | 32:DK:45:GLU:CB   | 2.47                     | 0.44              |
| 36:DO:39:VAL:HG12 | 36:DO:50:ALA:HB2  | 2.00                     | 0.44              |
| 37:DP:47:ILE:HG23 | 37:DP:63:ILE:CA   | 2.32                     | 0.44              |
| 38:DQ:64:ILE:C    | 38:DQ:66:ALA:N    | 2.75                     | 0.44              |
| 41:DT:14:PRO:HA   | 41:DT:32:LEU:HG   | 1.98                     | 0.44              |
| 42:DU:94:PHE:CD2  | 42:DU:95:PHE:N    | 2.84                     | 0.44              |
| 43:DW:19:ARG:NH2  | 43:DW:22:VAL:HA   | 2.32                     | 0.44              |
| 43:DW:57:THR:O    | 43:DW:58:LEU:C    | 2.59                     | 0.44              |
| 51:D4:14:CYS:SG   | 51:D4:26:ILE:HG23 | 2.57                     | 0.44              |
| 51:D4:15:LYS:C    | 51:D4:17:VAL:N    | 2.74                     | 0.44              |
| 1:AA:56:U:O5'     | 1:AA:56:U:H6      | 2.00                     | 0.44              |
| 1:AA:113:G:H2'    | 1:AA:114:U:H6     | 1.81                     | 0.44              |
| 1:AA:397:A:H3'    | 1:AA:397:A:N3     | 2.33                     | 0.44              |
| 1:AA:951:G:H1'    | 1:AA:970:C:O2'    | 2.17                     | 0.44              |
| 1:AA:1215:G:H5'   | 1:AA:1215:G:H8    | 1.80                     | 0.44              |
| 1:AA:1296:C:O2'   | 1:AA:1302:C:C2    | 2.71                     | 0.44              |
| 1:AA:1484:C:O2'   | 1:AA:1485:U:H5'   | 2.18                     | 0.44              |
| 3:AD:120:LYS:CB   | 3:AD:145:ARG:HH21 | 2.30                     | 0.44              |
| 6:AG:13:PRO:HB2   | 6:AG:18:GLY:C     | 2.42                     | 0.44              |
| 10:AK:92:ARG:NH1  | 21:AU:24:LYS:NZ   | 2.65                     | 0.44              |
| 11:AL:58:ASN:ND2  | 11:AL:60:PHE:HB2  | 2.33                     | 0.44              |
| 12:AM:75:SER:O    | 12:AM:78:ARG:HB3  | 2.17                     | 0.44              |
| 12:AM:78:ARG:HE   | 12:AM:79:LEU:CD1  | 2.29                     | 0.44              |
| 13:AN:24:ALA:HB1  | 13:AN:27:LYS:HZ1  | 1.82                     | 0.44              |
| 16:AQ:22:VAL:HG21 | 16:AQ:58:VAL:HG21 | 1.99                     | 0.44              |
| 17:AR:40:PRO:HD2  | 17:AR:43:ILE:HD11 | 1.98                     | 0.44              |
| 18:AS:16:LYS:O    | 18:AS:20:LYS:HB2  | 2.17                     | 0.44              |
| 20:AB:162:VAL:CG1 | 20:AB:184:ALA:HB2 | 2.47                     | 0.44              |
| 22:BA:49:C:OP2    | 36:BO:30:ARG:NH2  | 2.50                     | 0.44              |
| 23:BB:68:G:H2'    | 23:BB:68:G:N3     | 2.31                     | 0.44              |
| 23:BB:121:G:H4'   | 23:BB:149:A:H5'   | 2.00                     | 0.44              |
| 23:BB:144:A:H2'   | 23:BB:145:C:O4'   | 2.18                     | 0.44              |
| 23:BB:764:A:H5''  | 25:BC:208:GLY:HA3 | 1.98                     | 0.44              |
| 23:BB:770:G:OP1   | 49:B2:8:SER:HB2   | 2.17                     | 0.44              |
| 23:BB:863:A:H2'   | 23:BB:864:G:H8    | 1.83                     | 0.44              |
| 23:BB:956:G:H22   | 23:BB:959:A:H3'   | 1.80                     | 0.44              |
| 23:BB:966:G:H5''  | 23:BB:2272:U:O2   | 2.17                     | 0.44              |
| 23:BB:1164:C:H2'  | 23:BB:1165:A:C8   | 2.52                     | 0.44              |
| 23:BB:1189:A:H2'  | 23:BB:1190:G:O4'  | 2.17                     | 0.44              |
| 23:BB:1210:G:H4'  | 23:BB:1211:C:OP2  | 2.18                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:1228:G:H2'  | 23:BB:1229:C:H6    | 1.82                     | 0.44              |
| 23:BB:1346:G:C6   | 23:BB:1601:G:C6    | 3.05                     | 0.44              |
| 23:BB:1547:C:H2'  | 23:BB:1548:A:H8    | 1.81                     | 0.44              |
| 23:BB:1559:U:H3'  | 23:BB:1560:G:C5'   | 2.47                     | 0.44              |
| 23:BB:1785:A:H2'  | 23:BB:1787:A:C8    | 2.52                     | 0.44              |
| 23:BB:2393:U:OP1  | 50:B3:29:ARG:CZ    | 2.66                     | 0.44              |
| 23:BB:2604:U:O2'  | 23:BB:2605:U:H5'   | 2.17                     | 0.44              |
| 25:BC:103:ILE:CG2 | 25:BC:104:LEU:N    | 2.80                     | 0.44              |
| 25:BC:115:ILE:C   | 25:BC:116:GLN:HG3  | 2.42                     | 0.44              |
| 26:BD:23:PRO:HA   | 26:BD:190:LYS:CA   | 2.47                     | 0.44              |
| 26:BD:106:LYS:HE3 | 26:BD:106:LYS:HB2  | 1.77                     | 0.44              |
| 29:BG:16:VAL:HG21 | 29:BG:44:HIS:NE2   | 2.32                     | 0.44              |
| 29:BG:24:THR:OG1  | 29:BG:31:GLU:HB3   | 2.17                     | 0.44              |
| 30:BH:3:VAL:CG2   | 30:BH:21:VAL:HG11  | 2.44                     | 0.44              |
| 32:BK:35:VAL:HG23 | 32:BK:36:GLY:N     | 2.22                     | 0.44              |
| 35:BN:87:PHE:HB2  | 35:BN:94:TYR:CZ    | 2.52                     | 0.44              |
| 37:BP:1:SER:HB2   | 37:BP:4:ILE:HB     | 1.98                     | 0.44              |
| 39:BR:69:GLY:O    | 39:BR:70:GLU:HG3   | 2.17                     | 0.44              |
| 39:BR:78:ARG:HD3  | 39:BR:87:GLN:HG2   | 2.00                     | 0.44              |
| 40:BS:50:VAL:HG21 | 40:BS:103:ILE:HG21 | 1.98                     | 0.44              |
| 43:BW:48:ALA:HA   | 43:BW:54:ARG:HA    | 2.00                     | 0.44              |
| 43:BW:49:ASN:O    | 43:BW:50:VAL:HB    | 2.18                     | 0.44              |
| 1:CA:11:G:H2'     | 1:CA:12:U:C6       | 2.53                     | 0.44              |
| 1:CA:29:U:O2'     | 1:CA:30:U:H5'      | 2.17                     | 0.44              |
| 1:CA:36:C:H2'     | 1:CA:37:U:O4'      | 2.17                     | 0.44              |
| 1:CA:81:A:H2'     | 1:CA:82:G:H8       | 1.81                     | 0.44              |
| 1:CA:178:C:O2'    | 1:CA:179:A:H5'     | 2.18                     | 0.44              |
| 1:CA:668:G:O2'    | 1:CA:669:G:H5'     | 2.17                     | 0.44              |
| 2:CC:65:VAL:HG12  | 2:CC:65:VAL:O      | 2.17                     | 0.44              |
| 2:CC:87:ARG:HH11  | 2:CC:87:ARG:HG3    | 1.81                     | 0.44              |
| 3:CD:55:ARG:HH11  | 3:CD:55:ARG:CG     | 2.31                     | 0.44              |
| 3:CD:102:TYR:HE1  | 3:CD:108:ALA:O     | 2.01                     | 0.44              |
| 8:CI:30:ASN:HD21  | 8:CI:65:THR:C      | 2.26                     | 0.44              |
| 12:CM:21:ILE:O    | 12:CM:21:ILE:HG22  | 2.16                     | 0.44              |
| 13:CN:2:LYS:O     | 13:CN:3:GLN:C      | 2.60                     | 0.44              |
| 22:DA:49:C:H2'    | 22:DA:50:A:H8      | 1.83                     | 0.44              |
| 22:DA:99:A:N1     | 23:DB:863:A:H4'    | 2.33                     | 0.44              |
| 23:DB:7:G:H2'     | 23:DB:8:C:H6       | 1.82                     | 0.44              |
| 23:DB:20:C:H2'    | 23:DB:21:A:C8      | 2.51                     | 0.44              |
| 23:DB:145:C:H2'   | 23:DB:146:A:C8     | 2.52                     | 0.44              |
| 23:DB:182:A:H2    | 23:DB:433:C:O2     | 2.00                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:239:C:H2'    | 23:DB:240:C:C6     | 2.52                     | 0.44              |
| 23:DB:304:U:H2'    | 23:DB:305:C:H6     | 1.78                     | 0.44              |
| 23:DB:357:C:H2'    | 23:DB:358:U:H6     | 1.82                     | 0.44              |
| 23:DB:383:C:H5''   | 23:DB:385:C:OP2    | 2.17                     | 0.44              |
| 23:DB:538:A:N6     | 23:DB:555:G:O2'    | 2.43                     | 0.44              |
| 23:DB:814:C:H5''   | 39:DR:87:GLN:O     | 2.18                     | 0.44              |
| 23:DB:858:G:C2     | 23:DB:2268:A:H2'   | 2.47                     | 0.44              |
| 23:DB:1128:G:N7    | 23:DB:2490:G:H5'   | 2.32                     | 0.44              |
| 23:DB:1292:G:H2'   | 23:DB:1293:C:H6    | 1.83                     | 0.44              |
| 23:DB:2215:C:O2'   | 23:DB:2216:G:H5'   | 2.17                     | 0.44              |
| 23:DB:2377:A:H2    | 36:DO:92:PHE:HE1   | 1.65                     | 0.44              |
| 23:DB:2521:C:O2'   | 23:DB:2522:U:H5'   | 2.17                     | 0.44              |
| 23:DB:2669:G:H2'   | 23:DB:2670:A:C8    | 2.51                     | 0.44              |
| 23:DB:2758:A:H2'   | 23:DB:2759:G:C5'   | 2.45                     | 0.44              |
| 24:DV:72:VAL:CG1   | 24:DV:93:ARG:HA    | 2.42                     | 0.44              |
| 26:DD:83:ARG:HD2   | 26:DD:84:LEU:N     | 2.32                     | 0.44              |
| 26:DD:89:GLU:CD    | 26:DD:89:GLU:H     | 2.22                     | 0.44              |
| 26:DD:122:VAL:CG2  | 26:DD:128:ARG:HG3  | 2.46                     | 0.44              |
| 26:DD:202:ILE:HG22 | 26:DD:203:VAL:N    | 2.31                     | 0.44              |
| 27:DE:148:ILE:O    | 27:DE:148:ILE:HG13 | 2.17                     | 0.44              |
| 27:DE:151:GLY:HA2  | 27:DE:169:VAL:O    | 2.17                     | 0.44              |
| 29:DG:126:THR:C    | 29:DG:128:THR:H    | 2.24                     | 0.44              |
| 29:DG:156:TYR:CD1  | 29:DG:171:LYS:HG2  | 2.53                     | 0.44              |
| 33:DL:45:GLY:C     | 33:DL:47:ARG:N     | 2.74                     | 0.44              |
| 34:DM:33:LEU:CD2   | 34:DM:124:LEU:HD22 | 2.48                     | 0.44              |
| 37:DP:8:GLU:HA     | 37:DP:11:GLN:HG2   | 1.99                     | 0.44              |
| 39:DR:62:GLU:HB3   | 39:DR:103:ALA:C    | 2.43                     | 0.44              |
| 40:DS:18:ARG:NE    | 40:DS:22:ASP:OD1   | 2.50                     | 0.44              |
| 40:DS:22:ASP:O     | 40:DS:25:ARG:HG3   | 2.18                     | 0.44              |
| 47:D0:47:TYR:CD2   | 47:D0:51:ARG:HA    | 2.53                     | 0.44              |
| 51:D4:30:GLU:O     | 51:D4:32:LYS:N     | 2.50                     | 0.44              |
| 1:AA:613:C:H2'     | 1:AA:614:C:H6      | 1.82                     | 0.44              |
| 1:AA:915:A:C2'     | 1:AA:916:U:H5'     | 2.48                     | 0.44              |
| 1:AA:1148:U:H5''   | 8:AI:8:THR:HG23    | 2.00                     | 0.44              |
| 1:AA:1521:C:H2'    | 1:AA:1522:U:C6     | 2.53                     | 0.44              |
| 1:AA:1529:G:H3'    | 1:AA:1529:G:OP2    | 2.18                     | 0.44              |
| 2:AC:148:ILE:HA    | 2:AC:200:TRP:O     | 2.18                     | 0.44              |
| 3:AD:12:ARG:HD2    | 3:AD:37:PRO:HA     | 2.00                     | 0.44              |
| 3:AD:29:THR:C      | 3:AD:30:LYS:HD3    | 2.43                     | 0.44              |
| 3:AD:190:LEU:O     | 3:AD:192:ALA:N     | 2.50                     | 0.44              |
| 4:AE:105:ILE:HD12  | 4:AE:123:LEU:HB3   | 2.00                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:AI:4:GLN:NE2     | 8:AI:21:LYS:HE3   | 2.33                     | 0.44              |
| 9:AJ:57:VAL:HG22   | 9:AJ:58:ASN:H     | 1.83                     | 0.44              |
| 13:AN:17:ASP:HB2   | 13:AN:18:LYS:NZ   | 2.33                     | 0.44              |
| 13:AN:49:THR:HG22  | 13:AN:49:THR:O    | 2.17                     | 0.44              |
| 13:AN:63:CYS:HB2   | 13:AN:79:SER:OG   | 2.18                     | 0.44              |
| 14:AO:70:LYS:HZ1   | 14:AO:74:VAL:HA   | 1.83                     | 0.44              |
| 15:AP:78:VAL:O     | 15:AP:80:LYS:N    | 2.51                     | 0.44              |
| 18:AS:35:ARG:H     | 18:AS:35:ARG:HG3  | 1.50                     | 0.44              |
| 18:AS:47:THR:HG23  | 18:AS:60:PHE:HE1  | 1.83                     | 0.44              |
| 20:AB:9:LEU:H      | 20:AB:9:LEU:HD12  | 1.82                     | 0.44              |
| 23:BB:230:G:H2'    | 23:BB:231:A:H8    | 1.82                     | 0.44              |
| 23:BB:661:A:H2'    | 23:BB:662:G:H8    | 1.83                     | 0.44              |
| 23:BB:743:A:C2'    | 23:BB:744:U:H5'   | 2.47                     | 0.44              |
| 23:BB:985:C:H2'    | 23:BB:986:C:H6    | 1.83                     | 0.44              |
| 23:BB:1027:A:H2    | 23:BB:2488:G:H4'  | 1.82                     | 0.44              |
| 23:BB:1107:G:H2'   | 23:BB:1108:U:C6   | 2.53                     | 0.44              |
| 23:BB:1231:U:H2'   | 23:BB:1232:G:C8   | 2.52                     | 0.44              |
| 23:BB:1311:G:H21   | 23:BB:1603:A:H62  | 1.65                     | 0.44              |
| 23:BB:1535:A:H5'   | 23:BB:1536:C:C5   | 2.53                     | 0.44              |
| 23:BB:1561:C:H2'   | 23:BB:1562:U:H6   | 1.81                     | 0.44              |
| 23:BB:1669:A:C8    | 32:BK:5:GLN:HG3   | 2.53                     | 0.44              |
| 23:BB:1877:A:O2'   | 23:BB:1878:G:H5'  | 2.18                     | 0.44              |
| 23:BB:1910:G:O2'   | 23:BB:1911:U:H5'  | 2.18                     | 0.44              |
| 23:BB:1964:G:H4'   | 23:BB:1965:C:OP2  | 2.17                     | 0.44              |
| 23:BB:2150:C:H2'   | 23:BB:2151:U:O4'  | 2.17                     | 0.44              |
| 23:BB:2669:G:H2'   | 23:BB:2670:A:C8   | 2.51                     | 0.44              |
| 23:BB:2787:C:H2'   | 23:BB:2788:C:C6   | 2.53                     | 0.44              |
| 25:BC:6:LYS:HA     | 25:BC:7:PRO:HA    | 1.82                     | 0.44              |
| 25:BC:216:ARG:HB3  | 25:BC:217:PRO:HD2 | 1.99                     | 0.44              |
| 26:BD:29:VAL:HA    | 26:BD:185:ASN:OD1 | 2.18                     | 0.44              |
| 26:BD:40:LEU:O     | 26:BD:41:ALA:HB3  | 2.18                     | 0.44              |
| 26:BD:171:THR:HG22 | 26:BD:173:GLN:HG3 | 1.98                     | 0.44              |
| 27:BE:178:VAL:HG23 | 27:BE:179:SER:N   | 2.33                     | 0.44              |
| 28:BF:48:LEU:O     | 28:BF:49:LEU:HB2  | 2.17                     | 0.44              |
| 28:BF:116:LEU:H    | 28:BF:176:PHE:CA  | 2.31                     | 0.44              |
| 30:BH:134:VAL:HG22 | 30:BH:135:HIS:N   | 2.32                     | 0.44              |
| 32:BK:75:SER:N     | 37:BP:76:HIS:NE2  | 2.64                     | 0.44              |
| 33:BL:78:ARG:NH1   | 33:BL:80:SER:H    | 2.16                     | 0.44              |
| 40:BS:9:HIS:O      | 40:BS:10:ALA:HB3  | 2.18                     | 0.44              |
| 40:BS:70:LYS:CD    | 40:BS:110:ARG:HG3 | 2.47                     | 0.44              |
| 42:BU:2:ALA:O      | 42:BU:4:ILE:HG13  | 2.18                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:432:A:H2'    | 1:CA:433:G:H5'    | 1.99                     | 0.44              |
| 1:CA:949:A:O2'    | 1:CA:950:U:H5'    | 2.18                     | 0.44              |
| 1:CA:1142:G:H2'   | 1:CA:1143:G:O4'   | 2.17                     | 0.44              |
| 1:CA:1300:G:H2'   | 1:CA:1301:U:OP2   | 2.18                     | 0.44              |
| 1:CA:1349:A:H61   | 1:CA:1373:G:H1'   | 1.82                     | 0.44              |
| 1:CA:1414:U:H2'   | 1:CA:1415:G:C8    | 2.52                     | 0.44              |
| 1:CA:1425:U:H2'   | 1:CA:1426:G:C8    | 2.53                     | 0.44              |
| 3:CD:37:PRO:HD2   | 3:CD:41:GLY:CA    | 2.47                     | 0.44              |
| 3:CD:107:GLY:O    | 3:CD:157:ALA:HB1  | 2.17                     | 0.44              |
| 4:CE:68:ARG:O     | 4:CE:69:ASN:HB3   | 2.17                     | 0.44              |
| 5:CF:72:ASP:O     | 5:CF:75:GLU:HB3   | 2.18                     | 0.44              |
| 8:CI:6:TYR:OH     | 8:CI:8:THR:HG22   | 2.17                     | 0.44              |
| 9:CJ:68:ARG:HD3   | 9:CJ:70:HIS:CE1   | 2.53                     | 0.44              |
| 10:CK:12:ARG:CB   | 10:CK:13:LYS:HD2  | 2.47                     | 0.44              |
| 10:CK:84:MET:SD   | 10:CK:110:THR:OG1 | 2.73                     | 0.44              |
| 10:CK:117:HIS:O   | 10:CK:118:ASN:HB2 | 2.16                     | 0.44              |
| 11:CL:19:ASN:HB3  | 11:CL:85:ARG:HD2  | 1.99                     | 0.44              |
| 14:CO:42:PHE:CD1  | 14:CO:55:LEU:HD22 | 2.53                     | 0.44              |
| 18:CS:10:ILE:CG2  | 18:CS:40:PHE:HE2  | 2.31                     | 0.44              |
| 23:DB:11:C:H2'    | 23:DB:12:U:C5'    | 2.44                     | 0.44              |
| 23:DB:136:G:N2    | 41:DT:3:ARG:CZ    | 2.80                     | 0.44              |
| 23:DB:198:C:H5'   | 23:DB:2244:U:OP1  | 2.18                     | 0.44              |
| 23:DB:298:G:N2    | 23:DB:339:U:C5    | 2.86                     | 0.44              |
| 23:DB:319:G:H2'   | 23:DB:320:A:O4'   | 2.18                     | 0.44              |
| 23:DB:401:A:O2'   | 23:DB:402:A:C5'   | 2.65                     | 0.44              |
| 23:DB:1176:U:H2'  | 23:DB:1177:G:O4'  | 2.17                     | 0.44              |
| 23:DB:1341:G:C2'  | 23:DB:1397:U:O2'  | 2.66                     | 0.44              |
| 23:DB:1541:C:H2'  | 23:DB:1542:U:O4'  | 2.16                     | 0.44              |
| 23:DB:1589:U:H2'  | 23:DB:1590:A:C8   | 2.52                     | 0.44              |
| 23:DB:1659:G:C6   | 23:DB:2002:G:C6   | 3.06                     | 0.44              |
| 23:DB:1775:U:H2'  | 23:DB:1776:G:C5'  | 2.47                     | 0.44              |
| 23:DB:1785:A:H2'  | 23:DB:1787:A:C8   | 2.52                     | 0.44              |
| 23:DB:2294:G:OP2  | 36:DO:9:ARG:NE    | 2.49                     | 0.44              |
| 23:DB:2321:U:O2   | 23:DB:2321:U:O4'  | 2.35                     | 0.44              |
| 23:DB:2463:C:O2'  | 23:DB:2464:G:H5'  | 2.18                     | 0.44              |
| 23:DB:2533:U:H2'  | 23:DB:2534:A:O4'  | 2.17                     | 0.44              |
| 23:DB:2728:U:H2'  | 23:DB:2729:G:H8   | 1.82                     | 0.44              |
| 23:DB:2867:G:N3   | 23:DB:2867:G:C2'  | 2.73                     | 0.44              |
| 23:DB:2887:A:O4'  | 47:D0:27:LEU:HD11 | 2.17                     | 0.44              |
| 25:DC:23:LEU:HD12 | 25:DC:24:HIS:O    | 2.17                     | 0.44              |
| 25:DC:135:PRO:O   | 25:DC:165:ALA:HA  | 2.17                     | 0.44              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:DD:92:VAL:O     | 26:DD:93:GLY:C     | 2.60                     | 0.44              |
| 27:DE:1:MET:HE2    | 27:DE:1:MET:H2     | 1.82                     | 0.44              |
| 29:DG:93:TYR:HA    | 29:DG:105:SER:O    | 2.17                     | 0.44              |
| 29:DG:134:GLY:N    | 29:DG:140:ILE:HD11 | 2.32                     | 0.44              |
| 30:DH:4:ILE:H      | 30:DH:4:ILE:CD1    | 2.31                     | 0.44              |
| 30:DH:108:VAL:HG12 | 30:DH:110:VAL:CB   | 2.47                     | 0.44              |
| 33:DL:64:PHE:CD2   | 50:D3:11:LYS:HB3   | 2.49                     | 0.44              |
| 34:DM:5:LYS:HE3    | 34:DM:6:ARG:CA     | 2.45                     | 0.44              |
| 34:DM:119:LEU:HD22 | 34:DM:119:LEU:N    | 2.32                     | 0.44              |
| 35:DN:121:LYS:HD2  | 35:DN:122:ALA:H    | 1.83                     | 0.44              |
| 37:DP:34:GLY:O     | 37:DP:35:SER:HB3   | 2.17                     | 0.44              |
| 38:DQ:32:ARG:NH1   | 38:DQ:33:VAL:HG22  | 2.33                     | 0.44              |
| 40:DS:42:LYS:HE2   | 40:DS:45:VAL:HG21  | 1.99                     | 0.44              |
| 41:DT:9:LYS:HD3    | 44:DX:29:ARG:HH22  | 1.82                     | 0.44              |
| 51:D4:23:ILE:HD12  | 51:D4:24:ARG:HH11  | 1.82                     | 0.44              |
| 52:DI:76:ALA:O     | 52:DI:135:MET:HE1  | 2.18                     | 0.44              |
| 1:AA:206:C:H2'     | 1:AA:207:C:C6      | 2.53                     | 0.44              |
| 1:AA:500:G:H2'     | 1:AA:501:C:C6      | 2.53                     | 0.44              |
| 1:AA:1340:A:H2'    | 1:AA:1341:U:H6     | 1.81                     | 0.44              |
| 1:AA:1347:G:O2'    | 1:AA:1348:U:P      | 2.75                     | 0.44              |
| 2:AC:41:TYR:HA     | 2:AC:44:LYS:CD     | 2.47                     | 0.44              |
| 2:AC:77:GLY:CA     | 2:AC:81:GLU:HB3    | 2.46                     | 0.44              |
| 3:AD:39:GLN:HB3    | 3:AD:40:HIS:ND1    | 2.32                     | 0.44              |
| 3:AD:71:PHE:O      | 3:AD:74:TYR:HB2    | 2.17                     | 0.44              |
| 3:AD:177:MET:HE2   | 3:AD:177:MET:N     | 2.32                     | 0.44              |
| 5:AF:82:ASP:CG     | 25:BC:166:ARG:HH21 | 2.26                     | 0.44              |
| 7:AH:102:VAL:HG12  | 7:AH:125:ILE:HD12  | 1.99                     | 0.44              |
| 8:AI:24:ASN:C      | 8:AI:26:LYS:H      | 2.26                     | 0.44              |
| 10:AK:92:ARG:NH1   | 21:AU:24:LYS:HZ3   | 2.16                     | 0.44              |
| 10:AK:109:ILE:HG22 | 21:AU:16:ARG:HD2   | 1.99                     | 0.44              |
| 15:AP:6:LEU:HD12   | 15:AP:6:LEU:N      | 2.32                     | 0.44              |
| 16:AQ:39:ARG:HH11  | 16:AQ:39:ARG:CB    | 2.30                     | 0.44              |
| 20:AB:104:LYS:HE3  | 20:AB:104:LYS:HB2  | 1.82                     | 0.44              |
| 23:BB:43:G:H2'     | 23:BB:44:A:O4'     | 2.18                     | 0.44              |
| 23:BB:79:C:HO2'    | 23:BB:346:A:H1'    | 1.82                     | 0.44              |
| 23:BB:137:U:C2'    | 23:BB:138:U:H5'    | 2.48                     | 0.44              |
| 23:BB:197:A:H62    | 23:BB:2430:A:H2'   | 1.83                     | 0.44              |
| 23:BB:346:A:H3'    | 23:BB:347:A:H8     | 1.83                     | 0.44              |
| 23:BB:378:C:O2'    | 23:BB:379:G:H5'    | 2.17                     | 0.44              |
| 23:BB:443:A:C2     | 23:BB:1245:G:N3    | 2.86                     | 0.44              |
| 23:BB:456:C:H3'    | 41:BT:72:GLN:HE22  | 1.82                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:565:C:O2'    | 23:BB:566:U:H5'    | 2.18                     | 0.44              |
| 23:BB:1418:G:N2    | 23:BB:1579:A:C8    | 2.85                     | 0.44              |
| 23:BB:1509:A:C4'   | 23:BB:1510:G:H5'   | 2.48                     | 0.44              |
| 23:BB:1552:A:H2'   | 23:BB:1553:A:C5'   | 2.44                     | 0.44              |
| 23:BB:1724:G:H2'   | 23:BB:1725:U:H6    | 1.82                     | 0.44              |
| 23:BB:2206:C:O2'   | 23:BB:2207:C:H5'   | 2.17                     | 0.44              |
| 23:BB:2236:U:O2'   | 23:BB:2237:G:H5'   | 2.18                     | 0.44              |
| 23:BB:2508:G:O3'   | 23:BB:2555:U:H5'   | 2.18                     | 0.44              |
| 23:BB:2512:C:O2'   | 26:BD:146:ILE:CG1  | 2.66                     | 0.44              |
| 23:BB:2712:C:H2'   | 23:BB:2714:G:O3'   | 2.17                     | 0.44              |
| 24:BV:30:ILE:O     | 24:BV:37:PRO:HA    | 2.18                     | 0.44              |
| 25:BC:119:VAL:HG13 | 25:BC:133:ASN:CG   | 2.43                     | 0.44              |
| 25:BC:153:LEU:CD1  | 25:BC:161:VAL:HG23 | 2.47                     | 0.44              |
| 25:BC:237:ARG:HB2  | 25:BC:239:PHE:CE1  | 2.52                     | 0.44              |
| 27:BE:106:LYS:C    | 27:BE:108:ILE:N    | 2.76                     | 0.44              |
| 27:BE:148:ILE:N    | 27:BE:183:PHE:HB3  | 2.31                     | 0.44              |
| 28:BF:107:VAL:HB   | 28:BF:108:PRO:HD3  | 2.00                     | 0.44              |
| 29:BG:44:HIS:HB2   | 29:BG:49:LEU:HD23  | 2.00                     | 0.44              |
| 29:BG:125:PRO:HD2  | 29:BG:129:GLU:HB2  | 2.00                     | 0.44              |
| 31:BJ:71:ASP:O     | 31:BJ:72:LYS:HB2   | 2.17                     | 0.44              |
| 31:BJ:85:LYS:HA    | 31:BJ:85:LYS:HD3   | 1.77                     | 0.44              |
| 31:BJ:101:ILE:HG12 | 31:BJ:102:GLU:N    | 2.32                     | 0.44              |
| 34:BM:45:GLN:HE21  | 34:BM:119:LEU:HB3  | 1.81                     | 0.44              |
| 35:BN:9:GLN:HB2    | 35:BN:9:GLN:HE21   | 1.54                     | 0.44              |
| 36:BO:76:LYS:HB2   | 36:BO:106:LEU:HD13 | 1.99                     | 0.44              |
| 37:BP:18:SER:OG    | 37:BP:21:PRO:HD3   | 2.18                     | 0.44              |
| 39:BR:42:ALA:HA    | 39:BR:54:VAL:HG22  | 1.99                     | 0.44              |
| 39:BR:68:ARG:HD2   | 39:BR:70:GLU:OE1   | 2.17                     | 0.44              |
| 40:BS:17:VAL:HG23  | 40:BS:76:VAL:HG21  | 2.00                     | 0.44              |
| 40:BS:86:MET:HB2   | 40:BS:96:ILE:HD11  | 1.98                     | 0.44              |
| 41:BT:6:ARG:O      | 41:BT:8:LEU:N      | 2.50                     | 0.44              |
| 41:BT:15:HIS:HB2   | 41:BT:31:VAL:HG21  | 1.99                     | 0.44              |
| 41:BT:71:GLY:O     | 41:BT:72:GLN:HG3   | 2.17                     | 0.44              |
| 42:BU:11:ILE:O     | 42:BU:69:VAL:HB    | 2.18                     | 0.44              |
| 42:BU:13:LEU:N     | 42:BU:68:ASN:ND2   | 2.64                     | 0.44              |
| 43:BW:43:LYS:HA    | 43:BW:63:ASP:OD1   | 2.18                     | 0.44              |
| 43:BW:66:VAL:CG2   | 43:BW:67:LYS:H     | 2.26                     | 0.44              |
| 43:BW:66:VAL:O     | 43:BW:67:LYS:C     | 2.60                     | 0.44              |
| 46:BZ:63:ARG:NH2   | 46:BZ:66:ILE:HD12  | 2.33                     | 0.44              |
| 1:CA:86:G:O2'      | 1:CA:87:C:P        | 2.76                     | 0.44              |
| 1:CA:234:C:H2'     | 1:CA:235:C:C6      | 2.53                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:239:U:C5'     | 1:CA:239:U:C6      | 2.97                     | 0.44              |
| 1:CA:448:A:H2'     | 1:CA:449:G:C8      | 2.53                     | 0.44              |
| 1:CA:659:U:O2'     | 1:CA:660:C:H5'     | 2.18                     | 0.44              |
| 1:CA:695:A:C5'     | 10:CK:52:ARG:HH22  | 2.29                     | 0.44              |
| 1:CA:705:G:N2      | 10:CK:43:TRP:CE3   | 2.85                     | 0.44              |
| 1:CA:729:A:H2'     | 1:CA:730:G:H8      | 1.83                     | 0.44              |
| 1:CA:731:G:OP1     | 1:CA:766:A:H1'     | 2.16                     | 0.44              |
| 1:CA:1299:A:C5     | 1:CA:1301:U:H1'    | 2.53                     | 0.44              |
| 1:CA:1481:U:H2'    | 1:CA:1482:G:C8     | 2.52                     | 0.44              |
| 2:CC:156:LEU:CD1   | 2:CC:165:GLU:HB2   | 2.47                     | 0.44              |
| 3:CD:100:VAL:HG12  | 3:CD:101:VAL:N     | 2.33                     | 0.44              |
| 6:CG:78:ARG:HD2    | 6:CG:81:GLY:H      | 1.82                     | 0.44              |
| 7:CH:103:VAL:HG22  | 7:CH:124:ILE:HA    | 1.99                     | 0.44              |
| 15:CP:40:ASN:HD21  | 15:CP:42:ILE:CG1   | 2.30                     | 0.44              |
| 22:DA:92:C:H2'     | 22:DA:93:C:H6      | 1.82                     | 0.44              |
| 23:DB:435:C:H2'    | 23:DB:436:C:H5'    | 1.99                     | 0.44              |
| 23:DB:635:C:OP2    | 33:DL:126:ARG:NE   | 2.42                     | 0.44              |
| 23:DB:661:A:H2'    | 23:DB:662:G:H8     | 1.82                     | 0.44              |
| 23:DB:1027:A:N3    | 23:DB:2488:G:H5''  | 2.32                     | 0.44              |
| 23:DB:1028:A:N6    | 23:DB:1125:G:H2'   | 2.33                     | 0.44              |
| 23:DB:1117:C:C1'   | 34:DM:136:MET:HE1  | 2.48                     | 0.44              |
| 23:DB:1145:C:O2'   | 23:DB:1146:C:H5'   | 2.17                     | 0.44              |
| 23:DB:1529:G:H2'   | 23:DB:1530:G:C8    | 2.53                     | 0.44              |
| 23:DB:1746:A:H2'   | 23:DB:1747:U:C6    | 2.53                     | 0.44              |
| 23:DB:1985:C:O2'   | 23:DB:1986:C:H5'   | 2.17                     | 0.44              |
| 23:DB:2438:U:O2'   | 23:DB:2439:A:H5''  | 2.18                     | 0.44              |
| 25:DC:51:ARG:O     | 25:DC:51:ARG:HD3   | 2.17                     | 0.44              |
| 25:DC:182:LYS:HE2  | 25:DC:264:LYS:HZ2  | 1.83                     | 0.44              |
| 26:DD:180:VAL:HG23 | 26:DD:181:ASP:N    | 2.32                     | 0.44              |
| 27:DE:147:LEU:O    | 27:DE:148:ILE:HG13 | 2.18                     | 0.44              |
| 29:DG:42:VAL:HG23  | 29:DG:50:THR:C     | 2.42                     | 0.44              |
| 31:DJ:73:VAL:HG21  | 31:DJ:75:TYR:CE2   | 2.52                     | 0.44              |
| 31:DJ:94:ALA:CB    | 31:DJ:95:ARG:HH21  | 2.31                     | 0.44              |
| 33:DL:120:VAL:HG12 | 33:DL:122:VAL:HG22 | 1.98                     | 0.44              |
| 36:DO:79:ALA:O     | 36:DO:82:ALA:HB3   | 2.18                     | 0.44              |
| 40:DS:1:MET:HB3    | 40:DS:4:ILE:CD1    | 2.47                     | 0.44              |
| 40:DS:42:LYS:O     | 40:DS:45:VAL:HG22  | 2.17                     | 0.44              |
| 40:DS:84:ARG:HH21  | 40:DS:98:LYS:HZ1   | 1.66                     | 0.44              |
| 52:DI:138:VAL:HG12 | 52:DI:139:VAL:N    | 2.32                     | 0.44              |
| 1:AA:29:U:H5'      | 1:AA:296:U:OP1     | 2.17                     | 0.44              |
| 1:AA:993:G:C2'     | 1:AA:995:C:H41     | 2.31                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1001:C:H2'    | 1:AA:1002:G:C8     | 2.53                     | 0.44              |
| 1:AA:1050:G:O2'    | 1:AA:1051:C:H5'    | 2.18                     | 0.44              |
| 1:AA:1151:A:HO2'   | 1:AA:1152:A:H8     | 1.61                     | 0.44              |
| 1:AA:1264:U:O2'    | 1:AA:1265:C:H5'    | 2.17                     | 0.44              |
| 3:AD:32:LYS:O      | 3:AD:35:GLN:HB2    | 2.17                     | 0.44              |
| 5:AF:6:ILE:HB      | 5:AF:89:VAL:HB     | 2.00                     | 0.44              |
| 5:AF:41:ASP:OD1    | 5:AF:58:HIS:HE1    | 2.01                     | 0.44              |
| 5:AF:45:ARG:C      | 5:AF:56:LYS:HG2    | 2.42                     | 0.44              |
| 9:AJ:66:GLU:OE2    | 13:AN:98:ALA:HA    | 2.17                     | 0.44              |
| 12:AM:44:ILE:O     | 12:AM:47:LEU:HB2   | 2.17                     | 0.44              |
| 13:AN:11:LYS:O     | 13:AN:15:LEU:HG    | 2.18                     | 0.44              |
| 20:AB:160:LEU:HD23 | 20:AB:160:LEU:C    | 2.43                     | 0.44              |
| 23:BB:296:U:H2'    | 23:BB:297:G:C8     | 2.48                     | 0.44              |
| 23:BB:455:C:N3     | 23:BB:472:A:H2'    | 2.33                     | 0.44              |
| 23:BB:512:G:H4'    | 23:BB:512:G:OP1    | 2.18                     | 0.44              |
| 23:BB:675:A:O2'    | 27:BE:62:GLN:NE2   | 2.51                     | 0.44              |
| 23:BB:1110:G:N2    | 23:BB:1111:A:N6    | 2.66                     | 0.44              |
| 23:BB:1585:C:H2'   | 23:BB:1586:A:C8    | 2.52                     | 0.44              |
| 23:BB:1843:C:H2'   | 23:BB:1844:C:H6    | 1.81                     | 0.44              |
| 23:BB:2055:C:H4'   | 23:BB:2056:G:H5''  | 1.99                     | 0.44              |
| 23:BB:2070:A:H2'   | 23:BB:2071:A:O4'   | 2.18                     | 0.44              |
| 23:BB:2221:G:H2'   | 23:BB:2222:C:H6    | 1.83                     | 0.44              |
| 23:BB:2286:G:N3    | 23:BB:2286:G:H5'   | 2.33                     | 0.44              |
| 23:BB:2425:A:O2'   | 23:BB:2426:A:OP2   | 2.28                     | 0.44              |
| 23:BB:2431:U:O2'   | 23:BB:2433:A:N7    | 2.48                     | 0.44              |
| 23:BB:2601:C:C3'   | 23:BB:2602:A:H5''  | 2.48                     | 0.44              |
| 23:BB:2617:U:H2'   | 23:BB:2618:G:C5'   | 2.48                     | 0.44              |
| 23:BB:2733:A:H2'   | 23:BB:2734:A:O4'   | 2.17                     | 0.44              |
| 24:BV:79:ARG:NH1   | 24:BV:86:LEU:HD11  | 2.33                     | 0.44              |
| 25:BC:103:ILE:HG22 | 25:BC:104:LEU:H    | 1.81                     | 0.44              |
| 25:BC:114:GLN:HB2  | 25:BC:124:LYS:HZ2  | 1.81                     | 0.44              |
| 25:BC:140:VAL:HG23 | 25:BC:193:GLU:OE2  | 2.17                     | 0.44              |
| 26:BD:2:ILE:CG2    | 26:BD:204:LYS:HG3  | 2.48                     | 0.44              |
| 26:BD:88:GLU:HG2   | 26:BD:89:GLU:H     | 1.83                     | 0.44              |
| 27:BE:12:LEU:CD2   | 27:BE:118:LEU:HA   | 2.48                     | 0.44              |
| 29:BG:75:VAL:HG23  | 29:BG:76:ILE:N     | 2.31                     | 0.44              |
| 32:BK:63:VAL:HG13  | 32:BK:107:LEU:HD22 | 2.00                     | 0.44              |
| 33:BL:92:LEU:HG    | 33:BL:96:LYS:HZ3   | 1.82                     | 0.44              |
| 34:BM:8:LYS:O      | 34:BM:10:ARG:N     | 2.50                     | 0.44              |
| 35:BN:45:ARG:HD2   | 35:BN:45:ARG:H     | 1.82                     | 0.44              |
| 35:BN:68:ALA:C     | 35:BN:70:THR:H     | 2.26                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:BO:27:VAL:HA   | 36:BO:94:ARG:HB3   | 2.00                     | 0.44              |
| 37:BP:24:THR:HG21 | 37:BP:111:GLU:OE2  | 2.17                     | 0.44              |
| 37:BP:92:ARG:HB3  | 37:BP:110:LYS:O    | 2.18                     | 0.44              |
| 39:BR:41:ILE:HG12 | 39:BR:60:LYS:O     | 2.17                     | 0.44              |
| 39:BR:43:ASN:CG   | 39:BR:51:VAL:HB    | 2.43                     | 0.44              |
| 43:BW:71:LYS:O    | 43:BW:72:GLY:C     | 2.61                     | 0.44              |
| 52:BI:7:TYR:HB2   | 52:BI:59:THR:HA    | 1.99                     | 0.44              |
| 52:BI:11:GLN:NE2  | 52:BI:74:PRO:HG2   | 2.33                     | 0.44              |
| 1:CA:89:U:O2'     | 1:CA:90:C:H5'      | 2.17                     | 0.44              |
| 1:CA:109:A:C6     | 1:CA:326:G:C6      | 3.06                     | 0.44              |
| 1:CA:223:A:H2'    | 1:CA:224:U:C6      | 2.53                     | 0.44              |
| 1:CA:397:A:H3'    | 1:CA:397:A:N3      | 2.33                     | 0.44              |
| 1:CA:401:C:O2'    | 1:CA:402:G:H5'     | 2.18                     | 0.44              |
| 1:CA:500:G:H2'    | 1:CA:501:C:C6      | 2.53                     | 0.44              |
| 1:CA:542:G:O2'    | 1:CA:543:U:H5'     | 2.18                     | 0.44              |
| 1:CA:605:U:H2'    | 1:CA:606:G:C8      | 2.53                     | 0.44              |
| 1:CA:719:C:O2     | 17:CR:37:LYS:HA    | 2.18                     | 0.44              |
| 1:CA:947:G:H5''   | 12:CM:106:ARG:HB2  | 2.00                     | 0.44              |
| 1:CA:1172:C:O2'   | 1:CA:1173:U:H5'    | 2.17                     | 0.44              |
| 3:CD:137:SER:HB3  | 3:CD:138:PRO:HD2   | 2.00                     | 0.44              |
| 3:CD:169:TRP:CD1  | 3:CD:170:LEU:HG    | 2.53                     | 0.44              |
| 5:CF:30:THR:HA    | 5:CF:34:GLY:O      | 2.18                     | 0.44              |
| 5:CF:52:ASN:O     | 5:CF:53:LYS:HB3    | 2.17                     | 0.44              |
| 8:CI:5:TYR:O      | 8:CI:19:PHE:HB3    | 2.16                     | 0.44              |
| 8:CI:42:THR:HA    | 8:CI:45:MET:SD     | 2.57                     | 0.44              |
| 12:CM:95:PRO:HG2  | 12:CM:101:THR:HG22 | 1.98                     | 0.44              |
| 13:CN:71:GLY:O    | 13:CN:79:SER:HA    | 2.17                     | 0.44              |
| 14:CO:70:LYS:HB2  | 14:CO:77:TYR:CG    | 2.52                     | 0.44              |
| 18:CS:39:ILE:HD11 | 18:CS:70:LEU:HD13  | 2.00                     | 0.44              |
| 20:CB:72:LYS:O    | 20:CB:74:ALA:N     | 2.51                     | 0.44              |
| 23:DB:104:A:H2'   | 23:DB:105:C:C6     | 2.49                     | 0.44              |
| 23:DB:144:A:C5    | 41:DT:3:ARG:NH1    | 2.86                     | 0.44              |
| 23:DB:165:A:H2'   | 23:DB:166:U:C6     | 2.50                     | 0.44              |
| 23:DB:245:G:OP1   | 33:DL:67:THR:HB    | 2.18                     | 0.44              |
| 23:DB:619:G:H2'   | 23:DB:620:G:H5''   | 2.00                     | 0.44              |
| 23:DB:729:G:H4'   | 23:DB:763:G:C5'    | 2.47                     | 0.44              |
| 23:DB:1098:A:C8   | 52:DI:3:LYS:HB3    | 2.53                     | 0.44              |
| 23:DB:1171:G:N1   | 23:DB:1179:G:C6    | 2.85                     | 0.44              |
| 23:DB:1243:C:H1'  | 33:DL:14:LYS:HE3   | 2.00                     | 0.44              |
| 23:DB:1446:C:H2'  | 23:DB:1447:C:C6    | 2.52                     | 0.44              |
| 23:DB:1680:U:H2'  | 23:DB:1681:G:O4'   | 2.18                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:1802:A:C4'  | 25:DC:255:LYS:HE2  | 2.40                     | 0.44              |
| 24:DV:29:ILE:HG13 | 24:DV:30:ILE:N     | 2.33                     | 0.44              |
| 25:DC:251:THR:O   | 25:DC:252:LYS:CB   | 2.65                     | 0.44              |
| 26:DD:24:VAL:HG21 | 26:DD:193:VAL:HG13 | 2.00                     | 0.44              |
| 27:DE:58:LYS:HA   | 27:DE:59:PRO:HD3   | 1.66                     | 0.44              |
| 28:DF:35:LEU:HA   | 28:DF:153:ILE:HA   | 2.00                     | 0.44              |
| 29:DG:42:VAL:HG22 | 29:DG:43:LYS:N     | 2.33                     | 0.44              |
| 30:DH:5:LEU:HG    | 30:DH:13:GLY:C     | 2.42                     | 0.44              |
| 30:DH:104:THR:HA  | 30:DH:108:VAL:O    | 2.18                     | 0.44              |
| 30:DH:114:GLU:HB3 | 30:DH:133:GLN:NE2  | 2.25                     | 0.44              |
| 31:DJ:4:PHE:HD1   | 31:DJ:5:THR:N      | 2.16                     | 0.44              |
| 31:DJ:7:LYS:HD2   | 31:DJ:45:THR:HG21  | 1.99                     | 0.44              |
| 32:DK:2:ILE:HG23  | 32:DK:33:ALA:O     | 2.17                     | 0.44              |
| 40:DS:9:HIS:HA    | 40:DS:100:THR:OG1  | 2.18                     | 0.44              |
| 40:DS:56:ALA:O    | 40:DS:59:GLU:HB3   | 2.17                     | 0.44              |
| 40:DS:92:ARG:HH11 | 40:DS:92:ARG:HG2   | 1.82                     | 0.44              |
| 41:DT:15:HIS:O    | 41:DT:16:VAL:CB    | 2.66                     | 0.44              |
| 42:DU:8:ASP:HB2   | 42:DU:25:LYS:HE3   | 2.00                     | 0.44              |
| 43:DW:45:HIS:HE1  | 43:DW:71:LYS:HG3   | 1.81                     | 0.44              |
| 43:DW:81:ILE:HG23 | 43:DW:83:ALA:H     | 1.82                     | 0.44              |
| 45:DY:43:ILE:HA   | 45:DY:46:MET:CB    | 2.48                     | 0.44              |
| 52:DI:7:TYR:CZ    | 52:DI:57:VAL:HG11  | 2.52                     | 0.44              |
| 1:AA:11:G:H2'     | 1:AA:12:U:C6       | 2.52                     | 0.44              |
| 1:AA:15:G:O2'     | 4:AE:21:SER:HB2    | 2.17                     | 0.44              |
| 1:AA:432:A:H2'    | 1:AA:433:G:H5'     | 1.99                     | 0.44              |
| 1:AA:488:C:H2'    | 1:AA:489:C:C6      | 2.52                     | 0.44              |
| 1:AA:857:C:H2'    | 1:AA:858:G:O4'     | 2.17                     | 0.44              |
| 1:AA:989:U:O2'    | 1:AA:990:C:H5'     | 2.18                     | 0.44              |
| 1:AA:1049:U:C2'   | 13:AN:2:LYS:HD3    | 2.45                     | 0.44              |
| 1:AA:1172:C:H2'   | 1:AA:1173:U:H6     | 1.82                     | 0.44              |
| 2:AC:171:ARG:HH12 | 2:AC:173:PRO:HG3   | 1.83                     | 0.44              |
| 5:AF:38:ARG:CB    | 5:AF:63:ASN:HB2    | 2.37                     | 0.44              |
| 6:AG:144:ALA:C    | 6:AG:146:ALA:N     | 2.76                     | 0.44              |
| 8:AI:33:SER:HB3   | 8:AI:36:GLN:CB     | 2.43                     | 0.44              |
| 8:AI:43:ALA:HA    | 8:AI:44:ARG:HH12   | 1.82                     | 0.44              |
| 9:AJ:11:LYS:NZ    | 9:AJ:99:GLN:H      | 2.15                     | 0.44              |
| 9:AJ:36:VAL:HG22  | 9:AJ:76:ILE:HG22   | 1.99                     | 0.44              |
| 9:AJ:37:ARG:HB2   | 9:AJ:77:VAL:CG1    | 2.48                     | 0.44              |
| 11:AL:117:GLY:O   | 11:AL:118:VAL:HG13 | 2.18                     | 0.44              |
| 18:AS:44:ILE:HA   | 18:AS:61:VAL:CG1   | 2.48                     | 0.44              |
| 20:AB:90:PHE:CE2  | 20:AB:149:GLY:HA3  | 2.52                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 20:AB:131:LYS:O    | 20:AB:134:LEU:HB2 | 2.18                     | 0.44              |
| 20:AB:167:HIS:C    | 20:AB:169:HIS:H   | 2.25                     | 0.44              |
| 22:BA:45:A:O2'     | 22:BA:46:A:H5'    | 2.18                     | 0.44              |
| 22:BA:64:G:H2'     | 22:BA:65:U:C6     | 2.53                     | 0.44              |
| 23:BB:55:G:P       | 49:B2:35:ARG:HE   | 2.40                     | 0.44              |
| 23:BB:338:G:C2'    | 23:BB:339:U:H5'   | 2.48                     | 0.44              |
| 23:BB:340:A:C2'    | 23:BB:341:C:H5'   | 2.48                     | 0.44              |
| 23:BB:850:U:O2'    | 45:BY:21:ALA:HA   | 2.18                     | 0.44              |
| 23:BB:1080:A:H2'   | 23:BB:1081:U:C6   | 2.52                     | 0.44              |
| 23:BB:1152:C:H3'   | 55:BB:3244:HOH:O  | 2.17                     | 0.44              |
| 23:BB:1529:G:H2'   | 23:BB:1530:G:C8   | 2.52                     | 0.44              |
| 23:BB:1592:C:H2'   | 23:BB:1593:A:H8   | 1.83                     | 0.44              |
| 23:BB:1965:C:H3'   | 23:BB:1966:A:H8   | 1.83                     | 0.44              |
| 23:BB:2247:A:H3'   | 55:BB:3268:HOH:O  | 2.17                     | 0.44              |
| 23:BB:2305:U:N3    | 28:BF:150:GLY:HA3 | 2.33                     | 0.44              |
| 23:BB:2324:U:C5'   | 23:BB:2325:G:H5'' | 2.45                     | 0.44              |
| 23:BB:2335:A:OP2   | 36:BO:9:ARG:HA    | 2.18                     | 0.44              |
| 23:BB:2581:G:H2'   | 23:BB:2581:G:N3   | 2.33                     | 0.44              |
| 25:BC:128:THR:HG22 | 25:BC:129:LEU:H   | 1.83                     | 0.44              |
| 26:BD:31:ALA:O     | 26:BD:32:ASN:ND2  | 2.50                     | 0.44              |
| 26:BD:155:VAL:O    | 26:BD:156:PHE:HB2 | 2.18                     | 0.44              |
| 27:BE:40:ARG:HG2   | 27:BE:92:HIS:HB2  | 2.00                     | 0.44              |
| 27:BE:73:ILE:C     | 27:BE:75:SER:N    | 2.66                     | 0.44              |
| 27:BE:117:ARG:HA   | 27:BE:188:MET:SD  | 2.57                     | 0.44              |
| 27:BE:122:GLU:OE2  | 27:BE:152:GLU:HB2 | 2.18                     | 0.44              |
| 28:BF:89:THR:C     | 28:BF:90:LEU:HD12 | 2.42                     | 0.44              |
| 30:BH:30:LEU:O     | 30:BH:35:LYS:N    | 2.50                     | 0.44              |
| 30:BH:48:GLU:C     | 30:BH:50:ARG:N    | 2.74                     | 0.44              |
| 32:BK:26:GLY:HA3   | 32:BK:30:ARG:HG3  | 2.00                     | 0.44              |
| 33:BL:30:THR:HG22  | 33:BL:36:LYS:HZ2  | 1.79                     | 0.44              |
| 33:BL:38:GLN:CG    | 33:BL:39:LYS:H    | 2.26                     | 0.44              |
| 33:BL:56:PRO:HG3   | 33:BL:60:ARG:HH21 | 1.82                     | 0.44              |
| 35:BN:48:VAL:O     | 35:BN:52:ILE:HG12 | 2.18                     | 0.44              |
| 37:BP:38:ARG:CG    | 37:BP:39:LEU:H    | 2.28                     | 0.44              |
| 37:BP:54:LEU:HB3   | 37:BP:55:HIS:H    | 1.53                     | 0.44              |
| 39:BR:39:LEU:O     | 39:BR:54:VAL:HG11 | 2.17                     | 0.44              |
| 39:BR:43:ASN:OD1   | 39:BR:56:GLY:HA3  | 2.18                     | 0.44              |
| 39:BR:77:PHE:O     | 39:BR:78:ARG:HG3  | 2.17                     | 0.44              |
| 41:BT:31:VAL:O     | 41:BT:32:LEU:O    | 2.36                     | 0.44              |
| 42:BU:12:VAL:CG1   | 42:BU:18:LYS:H    | 2.31                     | 0.44              |
| 48:B1:10:LEU:CD1   | 48:B1:25:ASN:HD22 | 2.31                     | 0.44              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:28:A:O2'      | 1:CA:296:U:OP1     | 2.32                     | 0.44              |
| 1:CA:41:G:H2'      | 1:CA:42:G:H8       | 1.82                     | 0.44              |
| 1:CA:523:A:N1      | 11:CL:88:ASP:HB2   | 2.33                     | 0.44              |
| 1:CA:541:G:H2'     | 1:CA:542:G:C8      | 2.52                     | 0.44              |
| 1:CA:551:U:H2'     | 1:CA:552:U:C6      | 2.53                     | 0.44              |
| 1:CA:807:A:N3      | 25:DC:4:LYS:HE3    | 2.31                     | 0.44              |
| 1:CA:878:A:H5''    | 7:CH:80:PRO:HG2    | 2.00                     | 0.44              |
| 1:CA:1143:G:O2'    | 1:CA:1144:G:H5'    | 2.16                     | 0.44              |
| 1:CA:1333:A:H2'    | 1:CA:1334:G:O4'    | 2.17                     | 0.44              |
| 1:CA:1432:G:H1'    | 1:CA:1468:A:H61    | 1.81                     | 0.44              |
| 1:CA:1464:U:H2'    | 1:CA:1465:A:H8     | 1.83                     | 0.44              |
| 3:CD:84:ASN:HD21   | 3:CD:87:GLU:HG3    | 1.82                     | 0.44              |
| 4:CE:82:HIS:CE1    | 4:CE:146:MET:HB2   | 2.53                     | 0.44              |
| 6:CG:108:ARG:HG3   | 6:CG:108:ARG:HH11  | 1.83                     | 0.44              |
| 7:CH:10:LEU:HD22   | 7:CH:74:ILE:CD1    | 2.43                     | 0.44              |
| 9:CJ:37:ARG:N      | 9:CJ:76:ILE:HG12   | 2.33                     | 0.44              |
| 20:CB:21:TYR:O     | 20:CB:22:TRP:O     | 2.36                     | 0.44              |
| 23:DB:153:U:H2'    | 23:DB:154:U:C6     | 2.53                     | 0.44              |
| 23:DB:326:G:O2'    | 23:DB:327:G:H5'    | 2.17                     | 0.44              |
| 23:DB:630:G:H1     | 33:DL:69:ARG:HH12  | 1.64                     | 0.44              |
| 23:DB:844:A:H2     | 23:DB:845:A:N1     | 2.16                     | 0.44              |
| 23:DB:930:G:H5'    | 23:DB:931:U:P      | 2.57                     | 0.44              |
| 23:DB:998:C:H2'    | 23:DB:999:U:O4'    | 2.17                     | 0.44              |
| 23:DB:1252:G:H5''  | 55:DB:3462:HOH:O   | 2.18                     | 0.44              |
| 23:DB:1311:G:H21   | 23:DB:1603:A:H62   | 1.65                     | 0.44              |
| 23:DB:2061:G:H5''  | 23:DB:2503:A:N1    | 2.32                     | 0.44              |
| 23:DB:2313:C:H2'   | 23:DB:2314:A:C8    | 2.53                     | 0.44              |
| 23:DB:2556:C:O2'   | 23:DB:2557:G:H5'   | 2.17                     | 0.44              |
| 23:DB:2849:U:C4'   | 23:DB:2868:A:C2    | 3.01                     | 0.44              |
| 26:DD:180:VAL:HA   | 26:DD:187:LEU:HA   | 1.99                     | 0.44              |
| 26:DD:181:ASP:OD1  | 26:DD:184:ARG:HB3  | 2.17                     | 0.44              |
| 27:DE:139:LYS:HA   | 27:DE:143:LEU:HD23 | 1.98                     | 0.44              |
| 28:DF:8:LYS:HA     | 28:DF:12:VAL:CG2   | 2.48                     | 0.44              |
| 28:DF:120:SER:HB3  | 28:DF:127:TYR:HE1  | 1.83                     | 0.44              |
| 30:DH:45:GLU:HG3   | 30:DH:45:GLU:O     | 2.18                     | 0.44              |
| 31:DJ:73:VAL:CG2   | 31:DJ:74:TYR:N     | 2.81                     | 0.44              |
| 33:DL:19:LEU:O     | 33:DL:21:ARG:N     | 2.50                     | 0.44              |
| 33:DL:59:ARG:HH21  | 50:D3:5:THR:CB     | 2.30                     | 0.44              |
| 33:DL:101:ILE:HG22 | 33:DL:101:ILE:O    | 2.17                     | 0.44              |
| 34:DM:4:PRO:HB2    | 34:DM:69:PRO:HG3   | 1.99                     | 0.44              |
| 34:DM:16:ARG:O     | 34:DM:17:ASN:HB3   | 2.17                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:DN:103:ARG:HB3  | 35:DN:107:ASN:N   | 2.33                     | 0.44              |
| 36:DO:29:HIS:CB    | 36:DO:36:TYR:HB2  | 2.48                     | 0.44              |
| 38:DQ:111:LYS:HE2  | 39:DR:52:PRO:CG   | 2.45                     | 0.44              |
| 41:DT:61:LEU:HB3   | 41:DT:62:VAL:H    | 1.55                     | 0.44              |
| 41:DT:64:LYS:HE3   | 41:DT:64:LYS:N    | 2.33                     | 0.44              |
| 41:DT:76:ARG:HG2   | 41:DT:77:ARG:H    | 1.83                     | 0.44              |
| 45:DY:36:GLU:HG2   | 45:DY:37:ARG:N    | 2.32                     | 0.44              |
| 48:D1:12:SER:O     | 48:D1:13:SER:C    | 2.60                     | 0.44              |
| 52:DI:4:VAL:HG22   | 52:DI:5:GLN:N     | 2.33                     | 0.44              |
| 1:AA:542:G:O2'     | 1:AA:543:U:H5'    | 2.18                     | 0.44              |
| 1:AA:551:U:H2'     | 1:AA:552:U:C6     | 2.53                     | 0.44              |
| 1:AA:1248:A:H2     | 8:AI:71:ILE:HD11  | 1.82                     | 0.44              |
| 1:AA:1368:A:O2'    | 1:AA:1369:C:H5'   | 2.18                     | 0.44              |
| 1:AA:1520:C:H2'    | 1:AA:1521:C:C6    | 2.53                     | 0.44              |
| 3:AD:66:VAL:CG1    | 3:AD:70:GLN:HB3   | 2.47                     | 0.44              |
| 20:AB:58:LYS:CG    | 20:AB:62:ARG:HH21 | 2.26                     | 0.44              |
| 22:BA:54:G:O2'     | 22:BA:55:U:H5'    | 2.17                     | 0.44              |
| 22:BA:78:A:H61     | 22:BA:98:G:H1'    | 1.83                     | 0.44              |
| 22:BA:107:G:O2'    | 22:BA:108:A:H5'   | 2.18                     | 0.44              |
| 23:BB:106:C:H2'    | 23:BB:107:G:H8    | 1.83                     | 0.44              |
| 23:BB:465:G:H2'    | 23:BB:466:A:C8    | 2.52                     | 0.44              |
| 23:BB:499:U:H2'    | 23:BB:500:G:O4'   | 2.17                     | 0.44              |
| 23:BB:500:G:H1'    | 23:BB:505:A:N6    | 2.33                     | 0.44              |
| 23:BB:539:G:H2'    | 23:BB:540:C:C6    | 2.53                     | 0.44              |
| 23:BB:872:U:H1'    | 34:BM:68:PHE:CZ   | 2.53                     | 0.44              |
| 23:BB:992:C:H1'    | 39:BR:91:GLN:HB2  | 1.99                     | 0.44              |
| 23:BB:1072:C:N3    | 23:BB:1092:C:N4   | 2.65                     | 0.44              |
| 23:BB:1157:G:H2'   | 23:BB:1158:C:C6   | 2.53                     | 0.44              |
| 23:BB:1446:C:H2'   | 23:BB:1447:C:C6   | 2.52                     | 0.44              |
| 23:BB:2073:C:O2'   | 23:BB:2074:U:H5'  | 2.18                     | 0.44              |
| 23:BB:2438:U:O2'   | 23:BB:2439:A:H5'' | 2.18                     | 0.44              |
| 23:BB:2533:U:H2'   | 23:BB:2534:A:O4'  | 2.17                     | 0.44              |
| 25:BC:225:ASN:O    | 25:BC:227:VAL:N   | 2.51                     | 0.44              |
| 27:BE:97:ASN:HB2   | 27:BE:100:MET:HB2 | 1.99                     | 0.44              |
| 27:BE:199:MET:HE2  | 27:BE:199:MET:N   | 2.33                     | 0.44              |
| 28:BF:16:MET:HA    | 28:BF:16:MET:HE2  | 1.99                     | 0.44              |
| 28:BF:116:LEU:H    | 28:BF:176:PHE:C   | 2.26                     | 0.44              |
| 30:BH:55:GLU:C     | 30:BH:57:LYS:N    | 2.76                     | 0.44              |
| 30:BH:62:LEU:O     | 30:BH:66:ASN:N    | 2.51                     | 0.44              |
| 31:BJ:37:ARG:HH21  | 31:BJ:110:PRO:HG3 | 1.83                     | 0.44              |
| 33:BL:122:VAL:HG22 | 33:BL:139:GLY:O   | 2.18                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 37:BP:83:ILE:HG22 | 37:BP:84:SER:N    | 2.33                     | 0.44              |
| 37:BP:89:GLY:O    | 37:BP:90:ALA:C    | 2.60                     | 0.44              |
| 40:BS:48:LYS:O    | 40:BS:52:GLU:HG3  | 2.18                     | 0.44              |
| 41:BT:62:VAL:O    | 41:BT:63:VAL:O    | 2.35                     | 0.44              |
| 41:BT:68:LYS:HE3  | 41:BT:73:ARG:HG3  | 1.99                     | 0.44              |
| 43:BW:34:SER:OG   | 43:BW:39:GLN:NE2  | 2.51                     | 0.44              |
| 48:B1:42:VAL:HG12 | 48:B1:43:ARG:N    | 2.33                     | 0.44              |
| 50:B3:11:LYS:C    | 50:B3:12:ARG:HG3  | 2.42                     | 0.44              |
| 50:B3:57:VAL:HG13 | 50:B3:58:ILE:N    | 2.32                     | 0.44              |
| 52:BI:19:PRO:HG2  | 52:BI:22:PRO:HB2  | 2.00                     | 0.44              |
| 52:BI:72:THR:HB   | 52:BI:73:PRO:HD2  | 1.99                     | 0.44              |
| 1:CA:16:A:O2'     | 4:CE:20:VAL:HG23  | 2.18                     | 0.44              |
| 1:CA:56:U:H6      | 1:CA:56:U:O5'     | 2.00                     | 0.44              |
| 1:CA:57:G:N2      | 1:CA:388:G:C6     | 2.86                     | 0.44              |
| 1:CA:372:C:C1'    | 1:CA:373:A:OP2    | 2.66                     | 0.44              |
| 1:CA:617:G:C5'    | 15:CP:46:LYS:HD3  | 2.48                     | 0.44              |
| 1:CA:649:A:H2'    | 1:CA:650:G:O4'    | 2.17                     | 0.44              |
| 2:CC:95:GLY:C     | 2:CC:96:VAL:HG22  | 2.42                     | 0.44              |
| 3:CD:197:HIS:O    | 3:CD:200:VAL:HG12 | 2.17                     | 0.44              |
| 5:CF:99:ALA:O     | 5:CF:100:SER:HB2  | 2.18                     | 0.44              |
| 8:CI:62:LEU:HD22  | 8:CI:62:LEU:H     | 1.83                     | 0.44              |
| 10:CK:82:GLU:CB   | 10:CK:108:ASN:HB3 | 2.48                     | 0.44              |
| 11:CL:20:VAL:HA   | 11:CL:94:TYR:HE2  | 1.83                     | 0.44              |
| 13:CN:55:SER:OG   | 13:CN:56:PRO:HD2  | 2.18                     | 0.44              |
| 16:CQ:23:ALA:HB1  | 16:CQ:40:THR:CG2  | 2.48                     | 0.44              |
| 17:CR:28:LEU:C    | 17:CR:30:ASN:N    | 2.76                     | 0.44              |
| 20:CB:86:CYS:HB3  | 20:CB:88:GLN:CD   | 2.43                     | 0.44              |
| 20:CB:218:ALA:C   | 20:CB:220:VAL:N   | 2.76                     | 0.44              |
| 22:DA:22:U:H2'    | 22:DA:23:G:H8     | 1.75                     | 0.44              |
| 22:DA:29:A:OP1    | 22:DA:29:A:H8     | 2.01                     | 0.44              |
| 23:DB:138:U:O3'   | 23:DB:139:U:H3'   | 2.17                     | 0.44              |
| 23:DB:323:C:C5    | 27:DE:165:HIS:HB2 | 2.53                     | 0.44              |
| 23:DB:502:A:N6    | 23:DB:505:A:N1    | 2.66                     | 0.44              |
| 23:DB:1057:A:C8   | 23:DB:1086:A:C8   | 3.05                     | 0.44              |
| 23:DB:1157:G:N3   | 45:DY:10:ARG:NH2  | 2.66                     | 0.44              |
| 23:DB:1547:C:H2'  | 23:DB:1548:A:H8   | 1.81                     | 0.44              |
| 23:DB:1710:G:H2'  | 23:DB:1711:A:H8   | 1.83                     | 0.44              |
| 23:DB:1965:C:H3'  | 23:DB:1966:A:H8   | 1.83                     | 0.44              |
| 23:DB:2201:G:O2'  | 23:DB:2202:U:H5'  | 2.17                     | 0.44              |
| 23:DB:2604:U:O2'  | 23:DB:2605:U:H5'  | 2.17                     | 0.44              |
| 23:DB:2643:G:H2'  | 23:DB:2644:G:O4'  | 2.18                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:2787:C:H2'   | 23:DB:2788:C:C6    | 2.53                     | 0.44              |
| 23:DB:2811:G:H2'   | 23:DB:2812:G:H8    | 1.83                     | 0.44              |
| 25:DC:22:GLU:HB2   | 25:DC:202:ARG:HG3  | 1.99                     | 0.44              |
| 26:DD:5:VAL:HG21   | 26:DD:28:GLU:HA    | 2.00                     | 0.44              |
| 26:DD:69:ALA:HB2   | 26:DD:91:THR:OG1   | 2.18                     | 0.44              |
| 26:DD:89:GLU:HG2   | 26:DD:93:GLY:CA    | 2.41                     | 0.44              |
| 27:DE:126:VAL:O    | 27:DE:126:VAL:HG13 | 2.18                     | 0.44              |
| 27:DE:151:GLY:O    | 27:DE:158:PHE:HE1  | 2.01                     | 0.44              |
| 27:DE:168:ASP:OD2  | 27:DE:170:ARG:HG2  | 2.18                     | 0.44              |
| 28:DF:107:VAL:CG1  | 28:DF:175:PRO:HG3  | 2.48                     | 0.44              |
| 29:DG:53:PRO:HG2   | 29:DG:61:TRP:CE3   | 2.52                     | 0.44              |
| 29:DG:72:ASN:O     | 29:DG:76:ILE:HG13  | 2.18                     | 0.44              |
| 30:DH:27:ARG:HH11  | 46:DZ:56:ARG:HD2   | 1.82                     | 0.44              |
| 30:DH:31:VAL:CB    | 30:DH:32:PRO:HD3   | 2.38                     | 0.44              |
| 30:DH:134:VAL:HG12 | 30:DH:134:VAL:O    | 2.18                     | 0.44              |
| 34:DM:133:LYS:CG   | 34:DM:134:THR:H    | 2.31                     | 0.44              |
| 35:DN:32:GLU:HG3   | 35:DN:33:ILE:H     | 1.80                     | 0.44              |
| 35:DN:112:TYR:HE2  | 47:D0:43:THR:HB    | 1.82                     | 0.44              |
| 40:DS:4:ILE:HA     | 40:DS:106:VAL:HG12 | 1.98                     | 0.44              |
| 40:DS:17:VAL:HG11  | 40:DS:103:ILE:CD1  | 2.48                     | 0.44              |
| 41:DT:31:VAL:HA    | 41:DT:84:TYR:HA    | 2.00                     | 0.44              |
| 41:DT:55:VAL:HG21  | 41:DT:86:THR:H     | 1.82                     | 0.44              |
| 41:DT:76:ARG:HD3   | 41:DT:76:ARG:N     | 2.33                     | 0.44              |
| 42:DU:9:GLU:HB3    | 42:DU:21:ARG:HG2   | 1.99                     | 0.44              |
| 44:DX:1:MET:N      | 44:DX:6:LEU:HG     | 2.33                     | 0.44              |
| 52:DI:21:PRO:HB2   | 52:DI:22:PRO:CD    | 2.43                     | 0.44              |
| 1:AA:234:C:H2'     | 1:AA:235:C:C6      | 2.53                     | 0.43              |
| 1:AA:847:G:H2'     | 1:AA:848:C:C6      | 2.52                     | 0.43              |
| 1:AA:960:U:H1'     | 1:AA:961:U:OP2     | 2.17                     | 0.43              |
| 1:AA:1378:C:O2     | 1:AA:1378:C:H2'    | 2.16                     | 0.43              |
| 3:AD:187:ARG:HG3   | 3:AD:188:SER:N     | 2.32                     | 0.43              |
| 5:AF:51:ILE:CD1    | 5:AF:86:ARG:HG3    | 2.48                     | 0.43              |
| 6:AG:142:ARG:CZ    | 6:AG:142:ARG:HB2   | 2.48                     | 0.43              |
| 8:AI:97:LEU:N      | 8:AI:97:LEU:HD22   | 2.33                     | 0.43              |
| 10:AK:35:ASP:CB    | 10:AK:41:LEU:HD11  | 2.48                     | 0.43              |
| 11:AL:6:LEU:HB3    | 16:AQ:33:TYR:CZ    | 2.52                     | 0.43              |
| 13:AN:20:PHE:HA    | 13:AN:24:ALA:CB    | 2.46                     | 0.43              |
| 20:AB:112:ARG:NH1  | 20:AB:112:ARG:HG3  | 2.32                     | 0.43              |
| 23:BB:30:G:H2'     | 23:BB:31:C:C6      | 2.53                     | 0.43              |
| 23:BB:661:A:O2'    | 33:BL:23:ILE:HG12  | 2.18                     | 0.43              |
| 23:BB:728:G:H4'    | 25:BC:12:ARG:NH2   | 2.33                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:855:G:H21   | 43:BW:23:LYS:CG    | 2.30                     | 0.43              |
| 23:BB:1599:U:C2   | 23:BB:1600:C:C5    | 3.06                     | 0.43              |
| 23:BB:1658:C:OP1  | 26:BD:136:ASN:CA   | 2.66                     | 0.43              |
| 23:BB:1659:G:C6   | 23:BB:2002:G:C6    | 3.06                     | 0.43              |
| 23:BB:1775:U:H2'  | 23:BB:1776:G:C5'   | 2.48                     | 0.43              |
| 23:BB:1779:U:OP2  | 23:BB:1784:A:N6    | 2.46                     | 0.43              |
| 23:BB:1914:C:H2'  | 23:BB:1915:U:O4'   | 2.17                     | 0.43              |
| 23:BB:2052:A:C5'  | 26:BD:148:GLN:O    | 2.65                     | 0.43              |
| 23:BB:2061:G:H3'  | 55:BB:3546:HOH:O   | 2.18                     | 0.43              |
| 23:BB:2231:U:OP1  | 46:BZ:28:VAL:HG12  | 2.17                     | 0.43              |
| 23:BB:2385:C:H2'  | 23:BB:2386:A:C8    | 2.53                     | 0.43              |
| 23:BB:2886:A:C2   | 23:BB:2887:A:N7    | 2.85                     | 0.43              |
| 24:BV:4:ILE:HD11  | 24:BV:61:LEU:HD12  | 2.00                     | 0.43              |
| 24:BV:79:ARG:H    | 24:BV:79:ARG:HG2   | 1.46                     | 0.43              |
| 25:BC:19:VAL:CG1  | 25:BC:20:ASN:H     | 2.20                     | 0.43              |
| 25:BC:128:THR:CA  | 25:BC:190:THR:HA   | 2.41                     | 0.43              |
| 26:BD:32:ASN:OD1  | 26:BD:73:VAL:HB    | 2.18                     | 0.43              |
| 29:BG:97:VAL:HG23 | 29:BG:124:CYS:SG   | 2.58                     | 0.43              |
| 29:BG:102:ILE:CG2 | 29:BG:104:LEU:HD11 | 2.48                     | 0.43              |
| 33:BL:115:GLU:OE1 | 33:BL:115:GLU:HA   | 2.17                     | 0.43              |
| 34:BM:8:LYS:O     | 34:BM:9:PHE:CD1    | 2.71                     | 0.43              |
| 34:BM:80:VAL:HG12 | 34:BM:81:ARG:HG2   | 2.00                     | 0.43              |
| 37:BP:38:ARG:O    | 37:BP:39:LEU:HB2   | 2.18                     | 0.43              |
| 39:BR:37:GLU:OE1  | 39:BR:62:GLU:HB2   | 2.18                     | 0.43              |
| 39:BR:46:GLU:O    | 39:BR:47:VAL:CB    | 2.66                     | 0.43              |
| 39:BR:90:ARG:NH1  | 39:BR:91:GLN:N     | 2.64                     | 0.43              |
| 39:BR:97:LYS:HD2  | 39:BR:97:LYS:HA    | 1.82                     | 0.43              |
| 42:BU:90:LYS:CD   | 42:BU:91:LYS:H     | 2.32                     | 0.43              |
| 44:BX:22:LEU:CA   | 44:BX:47:ARG:HH22  | 2.31                     | 0.43              |
| 46:BZ:59:ARG:HG2  | 46:BZ:62:LYS:HB2   | 1.99                     | 0.43              |
| 49:B2:12:ARG:C    | 49:B2:16:HIS:O     | 2.61                     | 0.43              |
| 50:B3:35:LYS:O    | 50:B3:36:ALA:HB3   | 2.16                     | 0.43              |
| 52:BI:83:ALA:CA   | 52:BI:100:ILE:HD11 | 2.48                     | 0.43              |
| 1:CA:236:A:H2'    | 1:CA:237:G:C8      | 2.53                     | 0.43              |
| 1:CA:255:G:H2'    | 1:CA:256:U:C6      | 2.53                     | 0.43              |
| 1:CA:1211:U:H1'   | 1:CA:1213:A:C2     | 2.53                     | 0.43              |
| 1:CA:1463:U:H2'   | 1:CA:1464:U:C6     | 2.53                     | 0.43              |
| 2:CC:168:ARG:HE   | 2:CC:169:GLU:CA    | 2.30                     | 0.43              |
| 3:CD:121:ALA:CA   | 3:CD:145:ARG:HG3   | 2.48                     | 0.43              |
| 4:CE:88:HIS:CE1   | 4:CE:137:ARG:HH11  | 2.35                     | 0.43              |
| 4:CE:90:GLY:C     | 4:CE:129:SER:HB3   | 2.43                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:CF:48:ALA:H     | 17:CR:65:SER:HB2  | 1.82                     | 0.43              |
| 8:CI:27:ILE:CG2   | 8:CI:34:LEU:HB2   | 2.31                     | 0.43              |
| 8:CI:85:ALA:C     | 8:CI:87:MET:N     | 2.74                     | 0.43              |
| 10:CK:113:THR:CG2 | 21:CU:28:LEU:HD21 | 2.48                     | 0.43              |
| 11:CL:93:ARG:HD2  | 11:CL:93:ARG:N    | 2.29                     | 0.43              |
| 18:CS:30:LEU:HB2  | 18:CS:48:ILE:HA   | 2.00                     | 0.43              |
| 18:CS:39:ILE:HB   | 18:CS:66:VAL:O    | 2.18                     | 0.43              |
| 19:CT:17:ARG:HD2  | 19:CT:17:ARG:C    | 2.43                     | 0.43              |
| 20:CB:38:HIS:O    | 20:CB:39:ILE:HD13 | 2.17                     | 0.43              |
| 20:CB:218:ALA:C   | 20:CB:220:VAL:H   | 2.26                     | 0.43              |
| 23:DB:722:A:H2'   | 23:DB:723:C:O4'   | 2.18                     | 0.43              |
| 23:DB:946:C:H2'   | 23:DB:947:A:C8    | 2.48                     | 0.43              |
| 23:DB:1000:A:C8   | 23:DB:1154:G:N2   | 2.86                     | 0.43              |
| 23:DB:1346:G:C6   | 23:DB:1601:G:C6   | 3.05                     | 0.43              |
| 23:DB:1370:C:H2'  | 23:DB:1371:G:O4'  | 2.18                     | 0.43              |
| 23:DB:1418:G:N2   | 23:DB:1579:A:C8   | 2.86                     | 0.43              |
| 23:DB:1634:A:H3'  | 23:DB:1635:A:C5'  | 2.48                     | 0.43              |
| 23:DB:2250:G:N7   | 34:DM:82:MET:SD   | 2.91                     | 0.43              |
| 23:DB:2293:G:C5'  | 36:DO:9:ARG:HH21  | 2.31                     | 0.43              |
| 23:DB:2662:A:H2'  | 23:DB:2663:G:O4'  | 2.18                     | 0.43              |
| 23:DB:2787:C:H5'  | 26:DD:65:ALA:HB3  | 2.00                     | 0.43              |
| 24:DV:92:VAL:O    | 24:DV:92:VAL:HG13 | 2.18                     | 0.43              |
| 25:DC:179:GLU:CB  | 25:DC:266:ILE:HA  | 2.48                     | 0.43              |
| 26:DD:33:ARG:HD2  | 26:DD:89:GLU:OE2  | 2.17                     | 0.43              |
| 27:DE:73:ILE:HG22 | 27:DE:73:ILE:O    | 2.18                     | 0.43              |
| 27:DE:129:PRO:O   | 27:DE:130:LYS:HB2 | 2.18                     | 0.43              |
| 27:DE:142:ALA:C   | 27:DE:185:LYS:HZ2 | 2.25                     | 0.43              |
| 27:DE:147:LEU:HB3 | 27:DE:167:VAL:CG1 | 2.45                     | 0.43              |
| 27:DE:192:ALA:HB1 | 27:DE:199:MET:HG2 | 2.00                     | 0.43              |
| 31:DJ:41:LYS:HG2  | 38:DQ:63:ARG:CZ   | 2.48                     | 0.43              |
| 31:DJ:57:LEU:HG   | 31:DJ:128:ASN:C   | 2.43                     | 0.43              |
| 34:DM:97:GLN:H    | 34:DM:98:PRO:HD3  | 1.83                     | 0.43              |
| 36:DO:9:ARG:C     | 36:DO:11:ALA:N    | 2.75                     | 0.43              |
| 37:DP:49:ILE:HA   | 37:DP:62:LYS:O    | 2.18                     | 0.43              |
| 37:DP:100:ARG:HD2 | 37:DP:100:ARG:N   | 2.33                     | 0.43              |
| 40:DS:77:ASP:O    | 40:DS:101:SER:HB2 | 2.18                     | 0.43              |
| 48:D1:27:ARG:H    | 48:D1:27:ARG:HE   | 1.65                     | 0.43              |
| 1:AA:236:A:H2'    | 1:AA:237:G:C8     | 2.53                     | 0.43              |
| 1:AA:453:G:C6     | 1:AA:454:G:C6     | 3.06                     | 0.43              |
| 1:AA:1099:G:H2'   | 1:AA:1100:C:O4'   | 2.18                     | 0.43              |
| 1:AA:1424:U:H2'   | 1:AA:1425:U:H6    | 1.82                     | 0.43              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1437:A:O2'   | 1:AA:1438:G:H5'    | 2.18                     | 0.43              |
| 3:AD:6:PRO:HG3    | 3:AD:9:LYS:HD3     | 1.99                     | 0.43              |
| 3:AD:169:TRP:HB3  | 3:AD:183:ARG:HH21  | 1.84                     | 0.43              |
| 4:AE:14:LEU:HD13  | 4:AE:14:LEU:C      | 2.43                     | 0.43              |
| 4:AE:105:ILE:O    | 4:AE:123:LEU:HA    | 2.18                     | 0.43              |
| 6:AG:19:SER:HB2   | 6:AG:21:LEU:CD2    | 2.48                     | 0.43              |
| 8:AI:32:ARG:HH11  | 8:AI:32:ARG:HG2    | 1.84                     | 0.43              |
| 9:AJ:51:VAL:O     | 9:AJ:63:ASP:N      | 2.51                     | 0.43              |
| 10:AK:15:VAL:HG21 | 10:AK:41:LEU:CD1   | 2.49                     | 0.43              |
| 10:AK:110:THR:CG2 | 21:AU:4:LYS:HA     | 2.47                     | 0.43              |
| 11:AL:26:CYS:HB2  | 11:AL:29:LYS:HD3   | 2.01                     | 0.43              |
| 12:AM:103:THR:O   | 12:AM:104:ASN:C    | 2.61                     | 0.43              |
| 19:AT:50:PHE:HE2  | 19:AT:75:LYS:HA    | 1.83                     | 0.43              |
| 20:AB:150:ILE:CG1 | 20:AB:153:MET:HE3  | 2.46                     | 0.43              |
| 22:BA:32:U:H4'    | 22:BA:52:A:N6      | 2.33                     | 0.43              |
| 23:BB:396:G:O2'   | 46:BZ:28:VAL:HG11  | 2.18                     | 0.43              |
| 23:BB:409:G:O2'   | 23:BB:410:G:H5'    | 2.18                     | 0.43              |
| 23:BB:562:U:C4    | 23:BB:2036:C:O4'   | 2.71                     | 0.43              |
| 23:BB:850:U:H2'   | 23:BB:851:C:H6     | 1.82                     | 0.43              |
| 23:BB:877:A:H3'   | 23:BB:899:A:H61    | 1.82                     | 0.43              |
| 23:BB:1317:G:H2'  | 23:BB:1318:U:O4'   | 2.18                     | 0.43              |
| 23:BB:1341:G:C2'  | 23:BB:1397:U:O2'   | 2.66                     | 0.43              |
| 23:BB:1563:U:O2'  | 23:BB:1564:C:H5'   | 2.18                     | 0.43              |
| 23:BB:1683:U:O2'  | 23:BB:1684:G:H5'   | 2.18                     | 0.43              |
| 23:BB:1820:U:O2   | 25:BC:200:MET:HB2  | 2.17                     | 0.43              |
| 23:BB:1829:A:H3'  | 23:BB:1830:C:H6    | 1.83                     | 0.43              |
| 23:BB:2293:G:H2'  | 23:BB:2294:G:O4'   | 2.18                     | 0.43              |
| 25:BC:12:ARG:CZ   | 25:BC:18:VAL:HG11  | 2.48                     | 0.43              |
| 25:BC:68:ARG:NH1  | 25:BC:127:ASN:OD1  | 2.51                     | 0.43              |
| 25:BC:134:ILE:HA  | 25:BC:135:PRO:HD3  | 1.91                     | 0.43              |
| 25:BC:222:THR:HA  | 25:BC:231:HIS:CE1  | 2.53                     | 0.43              |
| 26:BD:3:GLY:CA    | 26:BD:49:GLN:HE22  | 2.32                     | 0.43              |
| 26:BD:114:LYS:HD3 | 35:BN:3:HIS:CE1    | 2.54                     | 0.43              |
| 26:BD:122:VAL:HB  | 26:BD:141:ARG:HH12 | 1.82                     | 0.43              |
| 26:BD:132:ALA:O   | 26:BD:136:ASN:N    | 2.51                     | 0.43              |
| 27:BE:3:LEU:HD21  | 27:BE:109:LEU:HD11 | 2.00                     | 0.43              |
| 27:BE:40:ARG:HD2  | 27:BE:43:THR:OG1   | 2.19                     | 0.43              |
| 28:BF:14:LYS:HG3  | 28:BF:15:LEU:N     | 2.32                     | 0.43              |
| 28:BF:67:THR:O    | 28:BF:83:PRO:HA    | 2.18                     | 0.43              |
| 28:BF:169:LEU:O   | 28:BF:173:ASP:OD1  | 2.36                     | 0.43              |
| 29:BG:148:ARG:CZ  | 29:BG:152:ARG:HB2  | 2.48                     | 0.43              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 30:BH:72:ILE:HD11  | 30:BH:75:LEU:HD12 | 1.99                     | 0.43              |
| 30:BH:142:VAL:HG12 | 30:BH:143:ILE:N   | 2.32                     | 0.43              |
| 32:BK:12:ASP:OD2   | 32:BK:85:VAL:HA   | 2.19                     | 0.43              |
| 35:BN:35:LYS:CA    | 35:BN:112:TYR:HB3 | 2.48                     | 0.43              |
| 37:BP:104:GLY:O    | 37:BP:105:LYS:HB3 | 2.18                     | 0.43              |
| 39:BR:42:ALA:HB1   | 39:BR:45:GLU:CD   | 2.43                     | 0.43              |
| 40:BS:33:LEU:HD22  | 40:BS:33:LEU:N    | 2.33                     | 0.43              |
| 41:BT:36:LYS:O     | 41:BT:81:LYS:HD2  | 2.17                     | 0.43              |
| 44:BX:8:GLU:CD     | 44:BX:8:GLU:C     | 2.85                     | 0.43              |
| 46:BZ:3:LYS:O      | 46:BZ:4:ASP:C     | 2.60                     | 0.43              |
| 52:BI:32:VAL:HG13  | 52:BI:66:PHE:CD2  | 2.53                     | 0.43              |
| 1:CA:60:A:HO2'     | 1:CA:61:G:C5'     | 2.32                     | 0.43              |
| 1:CA:488:C:H2'     | 1:CA:489:C:C6     | 2.52                     | 0.43              |
| 1:CA:695:A:H2'     | 1:CA:696:A:C8     | 2.53                     | 0.43              |
| 1:CA:908:A:O2'     | 1:CA:909:A:H5'    | 2.18                     | 0.43              |
| 1:CA:1051:C:H2'    | 1:CA:1052:U:C6    | 2.54                     | 0.43              |
| 1:CA:1080:A:C4'    | 4:CE:20:VAL:HG21  | 2.43                     | 0.43              |
| 1:CA:1092:A:H5''   | 6:CG:3:ARG:NH1    | 2.33                     | 0.43              |
| 1:CA:1236:A:H4'    | 1:CA:1304:G:H4'   | 2.01                     | 0.43              |
| 5:CF:19:PRO:HG2    | 5:CF:20:GLY:H     | 1.83                     | 0.43              |
| 8:CI:79:ARG:HA     | 8:CI:82:ILE:HD12  | 1.99                     | 0.43              |
| 10:CK:121:ARG:HH21 | 21:CU:34:ARG:CD   | 2.30                     | 0.43              |
| 13:CN:88:MET:HE2   | 13:CN:88:MET:HA   | 2.00                     | 0.43              |
| 15:CP:20:VAL:HG23  | 15:CP:34:GLU:C    | 2.43                     | 0.43              |
| 16:CQ:64:ARG:HG3   | 16:CQ:65:PRO:HD2  | 1.98                     | 0.43              |
| 21:CU:36:PHE:O     | 21:CU:37:TYR:C    | 2.61                     | 0.43              |
| 23:DB:268:C:O2     | 23:DB:268:C:H2'   | 2.17                     | 0.43              |
| 23:DB:285:G:C5     | 23:DB:356:G:C6    | 3.06                     | 0.43              |
| 23:DB:319:G:O2'    | 23:DB:320:A:H5'   | 2.18                     | 0.43              |
| 23:DB:515:A:H2     | 23:DB:1260:A:N3   | 2.16                     | 0.43              |
| 23:DB:557:C:O3'    | 31:DJ:113:PRO:HB2 | 2.18                     | 0.43              |
| 23:DB:1010:A:H5'   | 38:DQ:61:ILE:CG2  | 2.48                     | 0.43              |
| 23:DB:1221:C:H2'   | 23:DB:1222:U:C6   | 2.53                     | 0.43              |
| 23:DB:1261:C:C2'   | 23:DB:1262:A:O5'  | 2.67                     | 0.43              |
| 23:DB:1509:A:C4'   | 23:DB:1510:G:H5'  | 2.48                     | 0.43              |
| 23:DB:1561:C:H2'   | 23:DB:1562:U:H6   | 1.81                     | 0.43              |
| 23:DB:2457:U:C2'   | 23:DB:2458:G:H5'  | 2.48                     | 0.43              |
| 25:DC:42:ARG:CA    | 25:DC:42:ARG:NE   | 2.81                     | 0.43              |
| 27:DE:141:MET:HG3  | 27:DE:185:LYS:HE3 | 1.99                     | 0.43              |
| 27:DE:149:ILE:HD11 | 27:DE:188:MET:H   | 1.81                     | 0.43              |
| 28:DF:50:ASP:C     | 28:DF:52:ALA:N    | 2.75                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:DH:121:VAL:C   | 30:DH:123:ARG:H   | 2.24                     | 0.43              |
| 31:DJ:24:THR:O    | 31:DJ:28:LEU:HG   | 2.19                     | 0.43              |
| 34:DM:9:PHE:CE1   | 34:DM:11:LYS:HB2  | 2.54                     | 0.43              |
| 39:DR:92:TRP:CE3  | 39:DR:93:PHE:N    | 2.87                     | 0.43              |
| 41:DT:24:MET:HE3  | 41:DT:24:MET:H    | 1.82                     | 0.43              |
| 47:D0:29:VAL:HG22 | 47:D0:30:ASP:H    | 1.81                     | 0.43              |
| 52:DI:23:VAL:HG12 | 52:DI:24:GLY:H    | 1.83                     | 0.43              |
| 52:DI:73:PRO:HA   | 52:DI:74:PRO:HD3  | 1.92                     | 0.43              |
| 1:AA:12:U:H4'     | 1:AA:526:C:H4'    | 1.99                     | 0.43              |
| 1:AA:57:G:N2      | 1:AA:388:G:C6     | 2.86                     | 0.43              |
| 1:AA:90:C:H2'     | 1:AA:91:U:H6      | 1.83                     | 0.43              |
| 1:AA:113:G:N2     | 1:AA:353:A:H8     | 2.16                     | 0.43              |
| 1:AA:177:G:N3     | 1:AA:177:G:O4'    | 2.51                     | 0.43              |
| 1:AA:179:A:H2'    | 1:AA:180:U:C6     | 2.54                     | 0.43              |
| 1:AA:237:G:O2'    | 1:AA:238:A:H5'    | 2.18                     | 0.43              |
| 1:AA:429:U:H4'    | 1:AA:430:A:O5'    | 2.16                     | 0.43              |
| 1:AA:605:U:H2'    | 1:AA:606:G:C8     | 2.53                     | 0.43              |
| 1:AA:729:A:H2'    | 1:AA:730:G:H8     | 1.83                     | 0.43              |
| 1:AA:1113:C:O2'   | 1:AA:1114:C:H5'   | 2.17                     | 0.43              |
| 2:AC:21:TRP:CD1   | 2:AC:58:ARG:HD2   | 2.53                     | 0.43              |
| 2:AC:166:TRP:HB3  | 2:AC:167:TYR:H    | 1.45                     | 0.43              |
| 3:AD:51:GLY:O     | 3:AD:55:ARG:HB2   | 2.18                     | 0.43              |
| 3:AD:87:GLU:O     | 3:AD:88:ASN:C     | 2.61                     | 0.43              |
| 3:AD:194:ILE:HD11 | 3:AD:199:ILE:HD11 | 2.00                     | 0.43              |
| 11:AL:38:THR:CG2  | 11:AL:48:LEU:HD12 | 2.48                     | 0.43              |
| 14:AO:38:LEU:HB3  | 14:AO:42:PHE:HE1  | 1.83                     | 0.43              |
| 16:AQ:32:ILE:HG13 | 16:AQ:33:TYR:N    | 2.33                     | 0.43              |
| 16:AQ:60:ILE:HD13 | 16:AQ:60:ILE:H    | 1.83                     | 0.43              |
| 18:AS:7:GLY:O     | 18:AS:9:PHE:N     | 2.51                     | 0.43              |
| 18:AS:41:PRO:HG2  | 18:AS:42:ASN:H    | 1.83                     | 0.43              |
| 20:AB:73:ARG:C    | 20:AB:75:ALA:H    | 2.27                     | 0.43              |
| 23:BB:135:U:C2'   | 23:BB:136:G:C8    | 2.92                     | 0.43              |
| 23:BB:255:A:H2'   | 23:BB:256:A:O4'   | 2.18                     | 0.43              |
| 23:BB:540:C:H2'   | 23:BB:541:A:H8    | 1.83                     | 0.43              |
| 23:BB:711:G:H2'   | 23:BB:712:G:O4'   | 2.17                     | 0.43              |
| 23:BB:719:C:O2'   | 23:BB:720:U:H5'   | 2.18                     | 0.43              |
| 23:BB:725:G:H2'   | 23:BB:726:G:C1'   | 2.48                     | 0.43              |
| 23:BB:784:G:H5''  | 25:BC:225:ASN:ND2 | 2.33                     | 0.43              |
| 23:BB:975:A:N6    | 23:BB:989:G:O2'   | 2.52                     | 0.43              |
| 23:BB:1163:G:N2   | 39:BR:91:GLN:HG3  | 2.31                     | 0.43              |
| 23:BB:1290:C:O2'  | 23:BB:1291:C:H5'  | 2.19                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:BB:1364:G:N7    | 46:BZ:1:MET:HE1   | 2.33                     | 0.43              |
| 23:BB:1680:U:H2'   | 23:BB:1681:G:O4'  | 2.18                     | 0.43              |
| 23:BB:1710:G:H2'   | 23:BB:1711:A:H8   | 1.84                     | 0.43              |
| 23:BB:1812:U:H2'   | 23:BB:1813:G:C8   | 2.53                     | 0.43              |
| 23:BB:2014:A:OP1   | 40:BS:95:ARG:NE   | 2.39                     | 0.43              |
| 23:BB:2278:A:H62   | 43:BW:10:ARG:HG2  | 1.82                     | 0.43              |
| 23:BB:2289:G:O2'   | 23:BB:2290:G:H5'  | 2.18                     | 0.43              |
| 23:BB:2355:G:H4'   | 43:BW:20:LEU:CD2  | 2.45                     | 0.43              |
| 23:BB:2479:U:H6    | 23:BB:2479:U:O5'  | 2.01                     | 0.43              |
| 23:BB:2564:A:OP1   | 23:BB:2648:G:H4'  | 2.18                     | 0.43              |
| 23:BB:2728:U:H2'   | 23:BB:2729:G:H8   | 1.83                     | 0.43              |
| 23:BB:2866:U:O3'   | 23:BB:2867:G:H4'  | 2.18                     | 0.43              |
| 24:BV:82:TYR:HD1   | 34:BM:36:VAL:HB   | 1.83                     | 0.43              |
| 25:BC:33:LEU:HB3   | 25:BC:34:GLU:H    | 1.72                     | 0.43              |
| 25:BC:74:PRO:HB2   | 25:BC:96:LYS:CG   | 2.36                     | 0.43              |
| 25:BC:78:GLU:HB2   | 25:BC:92:LEU:HB3  | 1.99                     | 0.43              |
| 25:BC:171:VAL:HG12 | 25:BC:183:VAL:C   | 2.43                     | 0.43              |
| 26:BD:103:ASP:HA   | 26:BD:105:LYS:HE2 | 1.99                     | 0.43              |
| 27:BE:27:LEU:CD2   | 27:BE:100:MET:HG2 | 2.48                     | 0.43              |
| 27:BE:127:GLU:OE1  | 27:BE:130:LYS:HG3 | 2.19                     | 0.43              |
| 27:BE:139:LYS:HE2  | 27:BE:139:LYS:CA  | 2.48                     | 0.43              |
| 30:BH:60:GLU:OE1   | 30:BH:61:VAL:HG23 | 2.18                     | 0.43              |
| 30:BH:114:GLU:HB3  | 30:BH:134:VAL:HA  | 1.99                     | 0.43              |
| 30:BH:124:THR:HG22 | 30:BH:125:THR:H   | 1.82                     | 0.43              |
| 31:BJ:41:LYS:CD    | 31:BJ:44:TYR:HB2  | 2.45                     | 0.43              |
| 31:BJ:90:GLU:OE1   | 31:BJ:94:ALA:HB2  | 2.17                     | 0.43              |
| 32:BK:14:SER:O     | 32:BK:52:VAL:HB   | 2.18                     | 0.43              |
| 34:BM:67:VAL:O     | 34:BM:67:VAL:HG13 | 2.18                     | 0.43              |
| 34:BM:98:PRO:HG2   | 34:BM:99:GLY:H    | 1.83                     | 0.43              |
| 37:BP:22:GLY:HA3   | 37:BP:91:VAL:HG13 | 2.00                     | 0.43              |
| 37:BP:84:SER:O     | 37:BP:86:LYS:N    | 2.50                     | 0.43              |
| 44:BX:22:LEU:O     | 44:BX:23:ARG:C    | 2.61                     | 0.43              |
| 47:B0:51:ARG:NH1   | 47:B0:56:LYS:O    | 2.51                     | 0.43              |
| 52:BI:12:VAL:HG23  | 52:BI:41:PHE:CE2  | 2.53                     | 0.43              |
| 1:CA:374:A:H5''    | 1:CA:452:A:N1     | 2.33                     | 0.43              |
| 1:CA:402:G:H2'     | 1:CA:403:C:C6     | 2.53                     | 0.43              |
| 1:CA:797:C:OP1     | 10:CK:125:LYS:HE2 | 2.18                     | 0.43              |
| 1:CA:847:G:H2'     | 1:CA:848:C:C6     | 2.53                     | 0.43              |
| 1:CA:1187:G:OP1    | 8:CI:114:LYS:HE2  | 2.17                     | 0.43              |
| 1:CA:1301:U:HO2'   | 1:CA:1302:C:P     | 2.36                     | 0.43              |
| 1:CA:1458:G:O2'    | 1:CA:1459:G:H5'   | 2.19                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1460:C:O2'   | 1:CA:1461:G:H5'   | 2.19                     | 0.43              |
| 2:CC:8:GLY:HA2    | 2:CC:11:LEU:HG    | 1.99                     | 0.43              |
| 3:CD:179:GLY:O    | 3:CD:180:THR:HB   | 2.18                     | 0.43              |
| 4:CE:155:LYS:H    | 4:CE:155:LYS:HG3  | 1.53                     | 0.43              |
| 5:CF:9:MET:HE1    | 17:CR:64:LEU:O    | 2.18                     | 0.43              |
| 5:CF:43:GLY:HA2   | 5:CF:58:HIS:NE2   | 2.33                     | 0.43              |
| 8:CI:97:LEU:O     | 8:CI:102:PHE:HB2  | 2.17                     | 0.43              |
| 12:CM:56:ARG:HG3  | 12:CM:56:ARG:NH1  | 2.30                     | 0.43              |
| 14:CO:74:VAL:HG11 | 16:CQ:83:LEU:OXT  | 2.18                     | 0.43              |
| 22:DA:7:G:H4'     | 36:DO:29:HIS:CD2  | 2.53                     | 0.43              |
| 22:DA:114:C:H2'   | 22:DA:115:A:C8    | 2.53                     | 0.43              |
| 23:DB:192:C:O2'   | 23:DB:802:A:N3    | 2.51                     | 0.43              |
| 23:DB:908:C:O2'   | 23:DB:909:A:H5'   | 2.18                     | 0.43              |
| 23:DB:935:C:O2'   | 23:DB:936:A:H5'   | 2.18                     | 0.43              |
| 23:DB:947:A:H2'   | 23:DB:948:C:H6    | 1.76                     | 0.43              |
| 23:DB:1180:U:O2'  | 23:DB:1181:U:H5'  | 2.18                     | 0.43              |
| 23:DB:1236:G:H2'  | 23:DB:1237:A:OP2  | 2.18                     | 0.43              |
| 23:DB:1535:A:H5'  | 23:DB:1536:C:C5   | 2.52                     | 0.43              |
| 23:DB:1736:U:H2'  | 23:DB:1737:G:C8   | 2.52                     | 0.43              |
| 23:DB:1877:A:O2'  | 23:DB:1878:G:H5'  | 2.18                     | 0.43              |
| 23:DB:2259:U:N3   | 23:DB:2260:C:C5   | 2.86                     | 0.43              |
| 23:DB:2281:A:N6   | 43:DW:3:LYS:HE3   | 2.32                     | 0.43              |
| 23:DB:2310:C:H2'  | 23:DB:2311:A:H5'  | 1.99                     | 0.43              |
| 23:DB:2526:G:C2   | 51:D4:2:LYS:HE3   | 2.53                     | 0.43              |
| 23:DB:2530:A:H5'  | 29:DG:176:LYS:O   | 2.18                     | 0.43              |
| 23:DB:2733:A:C8   | 23:DB:2733:A:C3'  | 3.02                     | 0.43              |
| 25:DC:21:PRO:CD   | 25:DC:202:ARG:NH1 | 2.81                     | 0.43              |
| 26:DD:82:PHE:HB3  | 26:DD:83:ARG:H    | 1.42                     | 0.43              |
| 28:DF:7:TYR:OH    | 28:DF:29:ARG:HG2  | 2.18                     | 0.43              |
| 28:DF:140:ILE:C   | 28:DF:142:TYR:N   | 2.76                     | 0.43              |
| 31:DJ:95:ARG:N    | 31:DJ:95:ARG:NE   | 2.65                     | 0.43              |
| 31:DJ:120:ARG:HB3 | 31:DJ:121:LYS:CE  | 2.48                     | 0.43              |
| 32:DK:70:ARG:O    | 32:DK:70:ARG:HG3  | 2.18                     | 0.43              |
| 33:DL:61:LEU:HB3  | 33:DL:62:PRO:HD3  | 1.99                     | 0.43              |
| 37:DP:13:LYS:NZ   | 37:DP:15:ASP:HB2  | 2.33                     | 0.43              |
| 38:DQ:73:ILE:HG13 | 38:DQ:74:SER:N    | 2.22                     | 0.43              |
| 39:DR:20:VAL:HG12 | 39:DR:97:LYS:HA   | 1.99                     | 0.43              |
| 39:DR:38:VAL:HA   | 39:DR:61:ALA:HB3  | 1.99                     | 0.43              |
| 39:DR:58:VAL:O    | 39:DR:59:ILE:HB   | 2.17                     | 0.43              |
| 45:DY:3:THR:C     | 45:DY:36:GLU:HA   | 2.42                     | 0.43              |
| 1:AA:130:A:C8     | 16:AQ:64:ARG:HG3  | 2.53                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:195:A:H1'    | 1:AA:222:C:O2'     | 2.18                     | 0.43              |
| 1:AA:323:U:H4'    | 19:AT:16:ALA:HB3   | 2.01                     | 0.43              |
| 1:AA:340:U:H2'    | 1:AA:341:C:C6      | 2.54                     | 0.43              |
| 1:AA:392:C:H2'    | 1:AA:393:A:C8      | 2.54                     | 0.43              |
| 1:AA:462:G:H3'    | 1:AA:463:U:C5'     | 2.48                     | 0.43              |
| 1:AA:932:C:H5'    | 6:AG:3:ARG:NH2     | 2.34                     | 0.43              |
| 1:AA:1288:A:O2'   | 1:AA:1289:A:H5'    | 2.18                     | 0.43              |
| 2:AC:88:LYS:HD3   | 2:AC:88:LYS:C      | 2.42                     | 0.43              |
| 2:AC:113:LYS:HE2  | 2:AC:113:LYS:HA    | 2.00                     | 0.43              |
| 2:AC:147:GLY:HA3  | 2:AC:171:ARG:H     | 1.84                     | 0.43              |
| 7:AH:10:LEU:HA    | 7:AH:74:ILE:HD11   | 2.00                     | 0.43              |
| 8:AI:10:ARG:HA    | 8:AI:77:ALA:CB     | 2.49                     | 0.43              |
| 8:AI:85:ALA:O     | 8:AI:88:GLU:HB2    | 2.18                     | 0.43              |
| 9:AJ:39:PRO:CB    | 9:AJ:74:VAL:HG22   | 2.48                     | 0.43              |
| 9:AJ:41:PRO:O     | 9:AJ:71:LEU:HD13   | 2.18                     | 0.43              |
| 10:AK:60:PHE:HA   | 10:AK:63:GLN:CD    | 2.44                     | 0.43              |
| 11:AL:41:PRO:CB   | 11:AL:88:ASP:HB3   | 2.48                     | 0.43              |
| 14:AO:46:LYS:HE3  | 14:AO:46:LYS:HB2   | 1.84                     | 0.43              |
| 20:AB:61:SER:HB3  | 20:AB:223:GLY:O    | 2.17                     | 0.43              |
| 22:BA:91:C:H2'    | 22:BA:92:C:H6      | 1.83                     | 0.43              |
| 23:BB:211:C:O2'   | 23:BB:212:G:H5'    | 2.18                     | 0.43              |
| 23:BB:507:A:OP1   | 23:BB:508:A:N7     | 2.52                     | 0.43              |
| 23:BB:709:U:H2'   | 23:BB:710:U:H6     | 1.84                     | 0.43              |
| 23:BB:1025:G:H1'  | 23:BB:1135:C:O5'   | 2.18                     | 0.43              |
| 23:BB:1081:U:H4'  | 52:BI:123:ALA:HB1  | 2.01                     | 0.43              |
| 23:BB:1178:C:C2   | 23:BB:1179:G:N7    | 2.87                     | 0.43              |
| 23:BB:1183:U:C2   | 23:BB:1184:U:C5    | 3.06                     | 0.43              |
| 23:BB:1463:C:H2'  | 23:BB:1464:G:H8    | 1.82                     | 0.43              |
| 23:BB:1667:G:O2'  | 23:BB:1991:U:O4    | 2.35                     | 0.43              |
| 23:BB:1930:G:C2'  | 23:BB:1931:U:OP2   | 2.67                     | 0.43              |
| 23:BB:2457:U:O2'  | 23:BB:2458:G:H5'   | 2.18                     | 0.43              |
| 23:BB:2733:A:C8   | 23:BB:2733:A:C3'   | 3.02                     | 0.43              |
| 23:BB:2849:U:C4'  | 23:BB:2868:A:C2    | 3.01                     | 0.43              |
| 25:BC:131:MET:HE1 | 25:BC:173:LEU:HD11 | 2.00                     | 0.43              |
| 25:BC:168:GLY:C   | 25:BC:170:TYR:H    | 2.24                     | 0.43              |
| 26:BD:38:LYS:C    | 26:BD:42:ASN:HD21  | 2.26                     | 0.43              |
| 26:BD:140:HIS:HB3 | 26:BD:141:ARG:H    | 1.62                     | 0.43              |
| 26:BD:164:GLN:HG2 | 26:BD:165:MET:H    | 1.83                     | 0.43              |
| 27:BE:141:MET:CG  | 27:BE:143:LEU:HB2  | 2.48                     | 0.43              |
| 27:BE:149:ILE:CD1 | 27:BE:186:VAL:HG13 | 2.48                     | 0.43              |
| 27:BE:161:ALA:O   | 27:BE:162:ARG:HD2  | 2.18                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:BF:103:ILE:HG13 | 28:BF:104:THR:H    | 1.83                     | 0.43              |
| 28:BF:126:ASN:N    | 28:BF:126:ASN:ND2  | 2.50                     | 0.43              |
| 29:BG:49:LEU:O     | 29:BG:50:THR:HG23  | 2.19                     | 0.43              |
| 29:BG:57:TYR:N     | 29:BG:57:TYR:CD1   | 2.86                     | 0.43              |
| 30:BH:40:THR:O     | 30:BH:41:LYS:C     | 2.61                     | 0.43              |
| 31:BJ:25:LEU:HB2   | 31:BJ:26:GLY:H     | 1.57                     | 0.43              |
| 31:BJ:64:VAL:HG11  | 31:BJ:68:LYS:CD    | 2.34                     | 0.43              |
| 33:BL:82:LEU:HD13  | 33:BL:83:ALA:H     | 1.81                     | 0.43              |
| 34:BM:64:TRP:CE3   | 34:BM:102:LEU:HD22 | 2.54                     | 0.43              |
| 34:BM:81:ARG:C     | 34:BM:83:GLY:H     | 2.24                     | 0.43              |
| 35:BN:8:ARG:HB3    | 35:BN:43:GLU:OE1   | 2.19                     | 0.43              |
| 35:BN:24:MET:O     | 35:BN:28:LEU:HD12  | 2.18                     | 0.43              |
| 35:BN:57:THR:HG21  | 35:BN:61:ALA:HB3   | 2.01                     | 0.43              |
| 35:BN:122:ALA:CB   | 47:B0:49:ARG:HH12  | 2.32                     | 0.43              |
| 36:BO:84:GLU:O     | 36:BO:87:ILE:HG12  | 2.18                     | 0.43              |
| 37:BP:59:THR:HG1   | 37:BP:76:HIS:CE1   | 2.36                     | 0.43              |
| 38:BQ:94:LEU:CB    | 39:BR:13:ARG:HG2   | 2.49                     | 0.43              |
| 41:BT:68:LYS:HB2   | 41:BT:68:LYS:HE2   | 1.82                     | 0.43              |
| 43:BW:38:ARG:C     | 43:BW:38:ARG:HE    | 2.25                     | 0.43              |
| 45:BY:15:ARG:HE    | 45:BY:15:ARG:CA    | 2.31                     | 0.43              |
| 45:BY:44:ARG:HD2   | 45:BY:44:ARG:C     | 2.44                     | 0.43              |
| 46:BZ:50:ASP:C     | 46:BZ:53:THR:HG22  | 2.43                     | 0.43              |
| 47:B0:30:ASP:CG    | 47:B0:31:LYS:N     | 2.77                     | 0.43              |
| 48:B1:36:LYS:HB3   | 48:B1:37:LYS:H     | 1.67                     | 0.43              |
| 52:BI:77:VAL:HG23  | 52:BI:78:LEU:N     | 2.33                     | 0.43              |
| 1:CA:25:C:H2'      | 1:CA:26:A:C8       | 2.54                     | 0.43              |
| 1:CA:94:G:H4'      | 1:CA:95:C:H5''     | 2.01                     | 0.43              |
| 1:CA:425:G:O2'     | 1:CA:426:U:H5'     | 2.19                     | 0.43              |
| 1:CA:512:U:O2'     | 1:CA:513:C:H5'     | 2.19                     | 0.43              |
| 1:CA:521:G:O2'     | 1:CA:522:C:H5'     | 2.17                     | 0.43              |
| 1:CA:1248:A:H2'    | 1:CA:1249:C:H6     | 1.83                     | 0.43              |
| 1:CA:1253:G:N1     | 1:CA:1285:A:N6     | 2.66                     | 0.43              |
| 1:CA:1320:C:N4     | 18:CS:36:ARG:HD2   | 2.30                     | 0.43              |
| 1:CA:1521:C:H2'    | 1:CA:1522:U:C6     | 2.53                     | 0.43              |
| 2:CC:11:LEU:HD22   | 2:CC:17:TRP:CD1    | 2.54                     | 0.43              |
| 3:CD:61:ARG:HG3    | 3:CD:66:VAL:O      | 2.19                     | 0.43              |
| 5:CF:59:TYR:N      | 5:CF:59:TYR:CD1    | 2.86                     | 0.43              |
| 6:CG:11:ILE:HG22   | 6:CG:12:LEU:N      | 2.33                     | 0.43              |
| 8:CI:29:ILE:CA     | 8:CI:64:ILE:HB     | 2.46                     | 0.43              |
| 11:CL:106:VAL:CG1  | 11:CL:109:ARG:HG3  | 2.48                     | 0.43              |
| 13:CN:80:ARG:HH11  | 13:CN:80:ARG:HG2   | 1.84                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 14:CO:28:VAL:HB   | 14:CO:80:LEU:HD11  | 1.99                     | 0.43              |
| 18:CS:19:GLU:HG3  | 18:CS:19:GLU:O     | 2.18                     | 0.43              |
| 19:CT:15:LYS:HD3  | 19:CT:15:LYS:HA    | 1.74                     | 0.43              |
| 20:CB:41:ASN:ND2  | 20:CB:44:LYS:HB2   | 2.32                     | 0.43              |
| 23:DB:51:G:H1'    | 23:DB:118:A:H61    | 1.82                     | 0.43              |
| 23:DB:78:U:H2'    | 23:DB:79:C:H6      | 1.82                     | 0.43              |
| 23:DB:136:G:N1    | 41:DT:3:ARG:CZ     | 2.81                     | 0.43              |
| 23:DB:138:U:O3'   | 23:DB:139:U:H2'    | 2.19                     | 0.43              |
| 23:DB:215:G:H4'   | 23:DB:216:A:OP1    | 2.17                     | 0.43              |
| 23:DB:743:A:C2'   | 23:DB:744:U:H5'    | 2.47                     | 0.43              |
| 23:DB:1826:G:OP1  | 25:DC:222:THR:HG22 | 2.18                     | 0.43              |
| 23:DB:2281:A:H62  | 43:DW:3:LYS:HD2    | 1.83                     | 0.43              |
| 23:DB:2304:G:H22  | 23:DB:2312:U:H3    | 1.66                     | 0.43              |
| 23:DB:2349:G:OP2  | 50:D3:41:ARG:HD3   | 2.17                     | 0.43              |
| 23:DB:2361:G:C5'  | 50:D3:27:ASN:HB2   | 2.48                     | 0.43              |
| 23:DB:2660:A:H2'  | 23:DB:2661:G:O4'   | 2.17                     | 0.43              |
| 23:DB:2727:A:O2'  | 32:DK:70:ARG:NH2   | 2.52                     | 0.43              |
| 25:DC:68:ARG:CZ   | 25:DC:127:ASN:HA   | 2.46                     | 0.43              |
| 26:DD:50:VAL:CG1  | 26:DD:75:ALA:HB3   | 2.46                     | 0.43              |
| 26:DD:77:ARG:HH11 | 26:DD:77:ARG:CB    | 2.30                     | 0.43              |
| 32:DK:109:SER:C   | 32:DK:111:LYS:H    | 2.25                     | 0.43              |
| 34:DM:73:ILE:HG13 | 34:DM:92:TRP:HB2   | 2.00                     | 0.43              |
| 35:DN:28:LEU:HD23 | 35:DN:48:VAL:HG11  | 2.00                     | 0.43              |
| 39:DR:1:MET:N     | 39:DR:47:VAL:HB    | 2.33                     | 0.43              |
| 42:DU:81:ARG:HG3  | 42:DU:92:VAL:HG21  | 1.99                     | 0.43              |
| 48:D1:9:LYS:CG    | 48:D1:24:LYS:HG2   | 2.49                     | 0.43              |
| 48:D1:49:LYS:HD2  | 48:D1:49:LYS:O     | 2.17                     | 0.43              |
| 51:D4:10:LEU:HD13 | 51:D4:25:VAL:HB    | 2.00                     | 0.43              |
| 51:D4:26:ILE:HG23 | 51:D4:27:CYS:N     | 2.21                     | 0.43              |
| 1:AA:109:A:C6     | 1:AA:326:G:C6      | 3.06                     | 0.43              |
| 1:AA:186:C:H2'    | 1:AA:187:G:O4'     | 2.18                     | 0.43              |
| 1:AA:224:U:H2'    | 1:AA:225:C:H6      | 1.82                     | 0.43              |
| 1:AA:255:G:H2'    | 1:AA:256:U:C6      | 2.53                     | 0.43              |
| 1:AA:598:U:H2'    | 1:AA:599:C:H6      | 1.82                     | 0.43              |
| 1:AA:635:A:H2'    | 1:AA:636:U:C6      | 2.53                     | 0.43              |
| 1:AA:1213:A:C6    | 1:AA:1215:G:H1'    | 2.54                     | 0.43              |
| 1:AA:1454:G:H2'   | 1:AA:1455:G:O4'    | 2.19                     | 0.43              |
| 2:AC:24:ASN:O     | 2:AC:25:THR:C      | 2.62                     | 0.43              |
| 2:AC:112:ALA:O    | 2:AC:113:LYS:C     | 2.61                     | 0.43              |
| 8:AI:24:ASN:C     | 8:AI:26:LYS:HZ2    | 2.27                     | 0.43              |
| 9:AJ:80:THR:HG22  | 9:AJ:81:GLU:N      | 2.29                     | 0.43              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 13:AN:79:SER:O     | 13:AN:80:ARG:C    | 2.62                     | 0.43              |
| 13:AN:93:PRO:O     | 13:AN:94:GLY:C    | 2.61                     | 0.43              |
| 15:AP:25:ARG:HD3   | 15:AP:25:ARG:H    | 1.83                     | 0.43              |
| 15:AP:51:ARG:HH12  | 15:AP:53:ASP:CG   | 2.27                     | 0.43              |
| 16:AQ:7:LEU:C      | 16:AQ:9:GLY:H     | 2.27                     | 0.43              |
| 17:AR:64:LEU:C     | 17:AR:66:LEU:H    | 2.27                     | 0.43              |
| 20:AB:38:HIS:O     | 20:AB:39:ILE:HD13 | 2.17                     | 0.43              |
| 20:AB:187:ASP:OD1  | 20:AB:188:THR:N   | 2.51                     | 0.43              |
| 21:AU:16:ARG:NH2   | 21:AU:24:LYS:HE2  | 2.33                     | 0.43              |
| 23:BB:142:A:H8     | 23:BB:142:A:OP2   | 2.01                     | 0.43              |
| 23:BB:234:U:H2'    | 23:BB:235:U:H6    | 1.84                     | 0.43              |
| 23:BB:440:C:H2'    | 23:BB:441:U:H6    | 1.82                     | 0.43              |
| 23:BB:466:A:H2'    | 23:BB:467:G:H5'   | 2.01                     | 0.43              |
| 23:BB:619:G:H2'    | 23:BB:620:G:H5''  | 2.00                     | 0.43              |
| 23:BB:822:G:H2'    | 23:BB:823:C:C6    | 2.53                     | 0.43              |
| 23:BB:904:G:H2'    | 23:BB:905:A:C8    | 2.52                     | 0.43              |
| 23:BB:958:U:H5'    | 34:BM:18:ARG:HH12 | 1.83                     | 0.43              |
| 23:BB:1132:U:C6    | 31:BJ:85:LYS:HE2  | 2.53                     | 0.43              |
| 23:BB:1201:U:H2'   | 23:BB:1202:G:H8   | 1.84                     | 0.43              |
| 23:BB:2093:G:H2'   | 23:BB:2094:A:H8   | 1.84                     | 0.43              |
| 23:BB:2303:G:H2'   | 23:BB:2304:G:H5'  | 2.00                     | 0.43              |
| 23:BB:2686:G:H2'   | 23:BB:2687:U:O4'  | 2.18                     | 0.43              |
| 24:BV:26:PHE:HB2   | 24:BV:27:PRO:HD2  | 2.00                     | 0.43              |
| 25:BC:71:ASP:OD2   | 25:BC:118:GLY:HA2 | 2.19                     | 0.43              |
| 25:BC:88:ALA:CB    | 25:BC:156:SER:HB3 | 2.42                     | 0.43              |
| 25:BC:110:LYS:CE   | 25:BC:111:ALA:H   | 2.27                     | 0.43              |
| 25:BC:161:VAL:N    | 25:BC:193:GLU:CD  | 2.76                     | 0.43              |
| 25:BC:191:LEU:HD22 | 25:BC:191:LEU:O   | 2.17                     | 0.43              |
| 25:BC:257:ARG:HA   | 25:BC:257:ARG:CZ  | 2.47                     | 0.43              |
| 26:BD:62:LYS:HE3   | 26:BD:63:PRO:HD2  | 2.01                     | 0.43              |
| 27:BE:109:LEU:HA   | 27:BE:117:ARG:HB3 | 2.00                     | 0.43              |
| 27:BE:121:VAL:HG12 | 27:BE:122:GLU:H   | 1.80                     | 0.43              |
| 27:BE:138:LEU:HD22 | 27:BE:144:GLU:HA  | 1.99                     | 0.43              |
| 29:BG:30:GLY:C     | 29:BG:31:GLU:HG3  | 2.43                     | 0.43              |
| 30:BH:7:ASP:O      | 30:BH:8:LYS:C     | 2.62                     | 0.43              |
| 30:BH:58:LEU:O     | 30:BH:62:LEU:HD12 | 2.19                     | 0.43              |
| 30:BH:62:LEU:HD21  | 30:BH:137:GLU:HG2 | 2.01                     | 0.43              |
| 33:BL:39:LYS:HB3   | 33:BL:46:VAL:HG13 | 1.99                     | 0.43              |
| 33:BL:118:THR:N    | 33:BL:119:PRO:HD3 | 2.33                     | 0.43              |
| 34:BM:80:VAL:HG12  | 34:BM:81:ARG:N    | 2.33                     | 0.43              |
| 34:BM:96:ILE:HD13  | 34:BM:96:ILE:C    | 2.43                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 37:BP:47:ILE:CA   | 37:BP:63:ILE:HG23 | 2.48                     | 0.43              |
| 37:BP:92:ARG:CZ   | 37:BP:110:LYS:HE2 | 2.46                     | 0.43              |
| 39:BR:33:VAL:HB   | 39:BR:35:PHE:HE2  | 1.82                     | 0.43              |
| 40:BS:43:ALA:O    | 40:BS:47:VAL:HG13 | 2.18                     | 0.43              |
| 41:BT:15:HIS:HB2  | 41:BT:31:VAL:HB   | 1.99                     | 0.43              |
| 41:BT:89:GLU:C    | 41:BT:91:GLN:H    | 2.26                     | 0.43              |
| 43:BW:15:SER:O    | 43:BW:16:GLU:HB3  | 2.17                     | 0.43              |
| 44:BX:46:VAL:C    | 44:BX:48:ARG:H    | 2.27                     | 0.43              |
| 46:BZ:49:ARG:O    | 46:BZ:50:ASP:HB3  | 2.18                     | 0.43              |
| 50:B3:21:PHE:CD1  | 50:B3:21:PHE:N    | 2.85                     | 0.43              |
| 52:BI:85:ILE:HD12 | 52:BI:87:SER:O    | 2.19                     | 0.43              |
| 1:CA:113:G:N2     | 1:CA:353:A:H8     | 2.16                     | 0.43              |
| 1:CA:128:G:O2'    | 1:CA:129:A:H5'    | 2.18                     | 0.43              |
| 1:CA:206:C:H2'    | 1:CA:207:C:C6     | 2.53                     | 0.43              |
| 1:CA:239:U:H5''   | 1:CA:239:U:H6     | 1.80                     | 0.43              |
| 1:CA:847:G:H2'    | 1:CA:848:C:H6     | 1.82                     | 0.43              |
| 1:CA:916:U:H2'    | 1:CA:917:G:C8     | 2.52                     | 0.43              |
| 1:CA:1210:C:H4'   | 1:CA:1214:C:C4    | 2.53                     | 0.43              |
| 1:CA:1234:C:H2'   | 1:CA:1235:U:H6    | 1.83                     | 0.43              |
| 1:CA:1280:A:O4'   | 9:CJ:43:PRO:HG3   | 2.18                     | 0.43              |
| 1:CA:1348:U:O2    | 1:CA:1348:U:H2'   | 2.18                     | 0.43              |
| 1:CA:1376:U:H2'   | 1:CA:1377:A:C8    | 2.54                     | 0.43              |
| 2:CC:137:VAL:HG13 | 2:CC:148:ILE:HG23 | 2.00                     | 0.43              |
| 3:CD:64:TYR:CD2   | 3:CD:93:LEU:HB2   | 2.54                     | 0.43              |
| 3:CD:123:MET:HB2  | 3:CD:127:ARG:O    | 2.19                     | 0.43              |
| 3:CD:171:GLU:OE2  | 3:CD:182:LYS:HE3  | 2.19                     | 0.43              |
| 4:CE:136:VAL:HG23 | 4:CE:137:ARG:H    | 1.83                     | 0.43              |
| 8:CI:29:ILE:O     | 8:CI:32:ARG:HB2   | 2.18                     | 0.43              |
| 17:CR:51:GLN:NE2  | 17:CR:54:LEU:HB2  | 2.33                     | 0.43              |
| 18:CS:29:PRO:HB3  | 18:CS:47:THR:HG22 | 2.01                     | 0.43              |
| 19:CT:73:ARG:HG3  | 19:CT:74:HIS:H    | 1.83                     | 0.43              |
| 20:CB:11:ALA:C    | 20:CB:13:VAL:H    | 2.27                     | 0.43              |
| 21:CU:17:ARG:HD2  | 21:CU:17:ARG:N    | 2.12                     | 0.43              |
| 22:DA:13:G:H1'    | 22:DA:69:G:N2     | 2.33                     | 0.43              |
| 22:DA:53:A:C2'    | 22:DA:54:G:H5'    | 2.49                     | 0.43              |
| 23:DB:79:C:O2'    | 23:DB:346:A:C8    | 2.68                     | 0.43              |
| 23:DB:184:C:H2'   | 23:DB:185:G:C8    | 2.51                     | 0.43              |
| 23:DB:303:G:C6    | 23:DB:315:G:C6    | 3.06                     | 0.43              |
| 23:DB:511:U:H4'   | 23:DB:1235:G:H4'  | 2.00                     | 0.43              |
| 23:DB:585:G:H2'   | 23:DB:1251:C:N4   | 2.33                     | 0.43              |
| 23:DB:599:A:H2'   | 23:DB:600:G:H8    | 1.83                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DB:773:U:O2'    | 25:DC:48:ILE:HG23 | 2.18                     | 0.43              |
| 23:DB:1038:G:H2'   | 23:DB:1039:A:C8   | 2.52                     | 0.43              |
| 23:DB:1309:G:C5'   | 49:D2:8:SER:H     | 2.30                     | 0.43              |
| 23:DB:1616:A:H4'   | 23:DB:1617:C:OP2  | 2.19                     | 0.43              |
| 23:DB:1774:C:O2    | 23:DB:1774:C:C2'  | 2.54                     | 0.43              |
| 23:DB:1948:G:C6    | 23:DB:1959:G:C6   | 3.06                     | 0.43              |
| 23:DB:2072:C:O2'   | 23:DB:2073:C:H5'  | 2.19                     | 0.43              |
| 23:DB:2096:C:H2'   | 23:DB:2097:A:C8   | 2.53                     | 0.43              |
| 23:DB:2382:G:O2'   | 50:D3:38:LYS:HE2  | 2.18                     | 0.43              |
| 23:DB:2617:U:H2'   | 23:DB:2618:G:C5'  | 2.47                     | 0.43              |
| 23:DB:2691:C:H2'   | 23:DB:2692:G:H8   | 1.84                     | 0.43              |
| 24:DV:10:LYS:HD2   | 24:DV:41:GLU:OE2  | 2.18                     | 0.43              |
| 24:DV:57:TYR:CE2   | 24:DV:77:VAL:HG21 | 2.53                     | 0.43              |
| 24:DV:60:VAL:HG12  | 24:DV:73:LYS:HG3  | 2.00                     | 0.43              |
| 26:DD:70:LYS:HB3   | 26:DD:70:LYS:NZ   | 2.32                     | 0.43              |
| 29:DG:18:ILE:O     | 29:DG:18:ILE:HG13 | 2.18                     | 0.43              |
| 29:DG:171:LYS:C    | 29:DG:171:LYS:HD2 | 2.43                     | 0.43              |
| 30:DH:46:PHE:O     | 30:DH:49:ALA:HB3  | 2.19                     | 0.43              |
| 30:DH:108:VAL:C    | 30:DH:110:VAL:H   | 2.25                     | 0.43              |
| 31:DJ:35:ARG:O     | 31:DJ:52:ASP:HB2  | 2.18                     | 0.43              |
| 31:DJ:81:ILE:O     | 31:DJ:82:GLY:C    | 2.62                     | 0.43              |
| 31:DJ:95:ARG:HH11  | 31:DJ:95:ARG:HG3  | 1.83                     | 0.43              |
| 32:DK:19:VAL:HB    | 32:DK:41:ILE:CG1  | 2.49                     | 0.43              |
| 33:DL:54:GLN:CB    | 33:DL:57:LEU:HD23 | 2.48                     | 0.43              |
| 33:DL:63:LYS:HE3   | 50:D3:29:ARG:HG3  | 2.00                     | 0.43              |
| 33:DL:126:ARG:HH11 | 33:DL:126:ARG:HG2 | 1.83                     | 0.43              |
| 35:DN:18:GLN:HE21  | 35:DN:18:GLN:HB2  | 1.55                     | 0.43              |
| 35:DN:103:ARG:NH1  | 35:DN:106:ASP:OD2 | 2.51                     | 0.43              |
| 38:DQ:87:VAL:HB    | 39:DR:54:VAL:CG2  | 2.40                     | 0.43              |
| 40:DS:58:ALA:HA    | 40:DS:62:ASP:HB3  | 2.00                     | 0.43              |
| 43:DW:56:HIS:CD2   | 43:DW:58:LEU:H    | 2.36                     | 0.43              |
| 45:DY:57:GLU:OE1   | 45:DY:57:GLU:O    | 2.36                     | 0.43              |
| 46:DZ:61:ASN:C     | 46:DZ:63:ARG:H    | 2.26                     | 0.43              |
| 48:D1:27:ARG:H     | 48:D1:27:ARG:NE   | 2.16                     | 0.43              |
| 50:D3:25:HIS:CE1   | 50:D3:46:LYS:HB2  | 2.53                     | 0.43              |
| 51:D4:18:LYS:O     | 51:D4:19:ARG:HG3  | 2.17                     | 0.43              |
| 52:DI:7:TYR:CE1    | 52:DI:57:VAL:HG11 | 2.53                     | 0.43              |
| 1:AA:65:A:N3       | 1:AA:65:A:C2'     | 2.76                     | 0.43              |
| 1:AA:77:A:H2'      | 1:AA:78:A:N7      | 2.34                     | 0.43              |
| 1:AA:695:A:H2'     | 1:AA:696:A:C8     | 2.54                     | 0.43              |
| 1:AA:1140:C:O2'    | 1:AA:1141:C:H5'   | 2.18                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1220:G:H2'   | 1:AA:1221:G:C8     | 2.52                     | 0.43              |
| 1:AA:1238:A:N3    | 1:AA:1241:G:H1'    | 2.34                     | 0.43              |
| 1:AA:1343:G:H2'   | 1:AA:1344:C:C6     | 2.54                     | 0.43              |
| 1:AA:1343:G:H2'   | 1:AA:1344:C:H6     | 1.83                     | 0.43              |
| 1:AA:1367:C:O2'   | 1:AA:1368:A:H5'    | 2.16                     | 0.43              |
| 2:AC:139:ASN:N    | 2:AC:139:ASN:HD22  | 2.16                     | 0.43              |
| 3:AD:36:ALA:C     | 3:AD:38:GLY:H      | 2.26                     | 0.43              |
| 3:AD:64:TYR:CD1   | 3:AD:64:TYR:N      | 2.87                     | 0.43              |
| 5:AF:32:ALA:CB    | 5:AF:70:VAL:HG11   | 2.49                     | 0.43              |
| 8:AI:43:ALA:HA    | 8:AI:44:ARG:NH1    | 2.34                     | 0.43              |
| 8:AI:66:VAL:CG2   | 8:AI:74:GLN:HG3    | 2.48                     | 0.43              |
| 9:AJ:65:TYR:C     | 13:AN:98:ALA:HB2   | 2.44                     | 0.43              |
| 10:AK:69:CYS:C    | 10:AK:71:ASP:N     | 2.70                     | 0.43              |
| 12:AM:33:LEU:HB3  | 12:AM:38:ILE:O     | 2.18                     | 0.43              |
| 23:BB:161:A:H62   | 23:BB:165:A:N6     | 2.10                     | 0.43              |
| 23:BB:315:G:H2'   | 23:BB:316:C:O4'    | 2.19                     | 0.43              |
| 23:BB:636:G:OP2   | 33:BL:128:THR:HG22 | 2.18                     | 0.43              |
| 23:BB:954:G:OP1   | 34:BM:17:ASN:HB2   | 2.19                     | 0.43              |
| 23:BB:1115:G:H2'  | 23:BB:1116:G:H8    | 1.83                     | 0.43              |
| 23:BB:1117:C:C2   | 23:BB:1118:C:C5    | 3.07                     | 0.43              |
| 23:BB:1155:A:H61  | 45:BY:10:ARG:CZ    | 2.31                     | 0.43              |
| 23:BB:1877:A:H2'  | 23:BB:1878:G:C8    | 2.53                     | 0.43              |
| 23:BB:1948:G:C6   | 23:BB:1959:G:C6    | 3.06                     | 0.43              |
| 23:BB:2184:A:H2'  | 23:BB:2185:U:C6    | 2.53                     | 0.43              |
| 23:BB:2210:U:N3   | 23:BB:2212:A:N7    | 2.65                     | 0.43              |
| 23:BB:2728:U:H2'  | 23:BB:2729:G:C8    | 2.54                     | 0.43              |
| 23:BB:2771:C:O2'  | 26:BD:173:GLN:NE2  | 2.52                     | 0.43              |
| 24:BV:42:LEU:N    | 24:BV:42:LEU:HD23  | 2.33                     | 0.43              |
| 25:BC:25:LYS:HA   | 25:BC:25:LYS:HD2   | 1.83                     | 0.43              |
| 25:BC:137:GLY:C   | 25:BC:139:THR:N    | 2.76                     | 0.43              |
| 25:BC:194:VAL:CG1 | 25:BC:195:GLY:H    | 2.17                     | 0.43              |
| 26:BD:24:VAL:O    | 26:BD:24:VAL:HG13  | 2.18                     | 0.43              |
| 26:BD:52:THR:HG22 | 26:BD:76:GLY:H     | 1.84                     | 0.43              |
| 27:BE:149:ILE:O   | 27:BE:187:VAL:HG22 | 2.18                     | 0.43              |
| 27:BE:150:THR:HB  | 27:BE:171:ASP:OD1  | 2.18                     | 0.43              |
| 28:BF:3:LEU:HA    | 28:BF:6:TYR:CG     | 2.54                     | 0.43              |
| 28:BF:45:ASP:OD2  | 28:BF:83:PRO:HG2   | 2.18                     | 0.43              |
| 28:BF:65:LEU:C    | 28:BF:67:THR:N     | 2.76                     | 0.43              |
| 31:BJ:35:ARG:NH2  | 31:BJ:40:HIS:H     | 2.15                     | 0.43              |
| 31:BJ:43:GLU:HG3  | 31:BJ:44:TYR:CD2   | 2.53                     | 0.43              |
| 32:BK:5:GLN:NE2   | 32:BK:20:MET:HE1   | 2.33                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:BM:71:LYS:HD3  | 34:BM:92:TRP:N     | 2.33                     | 0.43              |
| 34:BM:116:ALA:C   | 34:BM:119:LEU:HD23 | 2.43                     | 0.43              |
| 35:BN:41:ALA:C    | 35:BN:43:GLU:N     | 2.77                     | 0.43              |
| 37:BP:51:ASN:HA   | 37:BP:61:ARG:N     | 2.29                     | 0.43              |
| 38:BQ:92:LYS:O    | 38:BQ:94:LEU:HD22  | 2.18                     | 0.43              |
| 43:BW:45:HIS:HB2  | 43:BW:67:LYS:NZ    | 2.33                     | 0.43              |
| 44:BX:21:LEU:C    | 44:BX:23:ARG:H     | 2.26                     | 0.43              |
| 45:BY:23:LEU:HD22 | 45:BY:28:LEU:O     | 2.18                     | 0.43              |
| 46:BZ:32:LEU:HD22 | 46:BZ:32:LEU:C     | 2.43                     | 0.43              |
| 52:BI:15:GLY:O    | 52:BI:16:MET:HB2   | 2.16                     | 0.43              |
| 1:CA:177:G:N3     | 1:CA:177:G:O4'     | 2.51                     | 0.43              |
| 1:CA:302:G:H2'    | 1:CA:303:A:H8      | 1.83                     | 0.43              |
| 1:CA:409:U:OP2    | 3:CD:21:LYS:HE2    | 2.19                     | 0.43              |
| 1:CA:625:U:H4'    | 15:CP:16:PHE:CZ    | 2.54                     | 0.43              |
| 1:CA:1014:A:H5''  | 18:CS:13:HIS:HB2   | 2.00                     | 0.43              |
| 1:CA:1426:G:O2'   | 1:CA:1427:C:H5'    | 2.19                     | 0.43              |
| 1:CA:1455:G:O2'   | 1:CA:1456:A:H5'    | 2.18                     | 0.43              |
| 4:CE:87:VAL:CG1   | 4:CE:88:HIS:H      | 2.26                     | 0.43              |
| 8:CI:8:THR:OG1    | 8:CI:84:ARG:HG3    | 2.18                     | 0.43              |
| 8:CI:123:ARG:HD3  | 8:CI:124:PRO:HD2   | 1.99                     | 0.43              |
| 12:CM:100:ARG:C   | 12:CM:102:LYS:H    | 2.26                     | 0.43              |
| 20:CB:53:LEU:HD11 | 20:CB:216:VAL:HG12 | 1.99                     | 0.43              |
| 22:DA:53:A:H2'    | 22:DA:54:G:O4'     | 2.19                     | 0.43              |
| 23:DB:80:G:C6     | 23:DB:107:G:C6     | 3.07                     | 0.43              |
| 23:DB:852:U:H2'   | 23:DB:853:C:C6     | 2.53                     | 0.43              |
| 23:DB:948:C:O2'   | 23:DB:949:G:H5'    | 2.19                     | 0.43              |
| 23:DB:1092:C:O2'  | 23:DB:1093:G:H5'   | 2.19                     | 0.43              |
| 23:DB:1341:G:H5'  | 41:DT:61:LEU:CD2   | 2.44                     | 0.43              |
| 23:DB:1373:A:H5'' | 23:DB:2213:U:O4    | 2.18                     | 0.43              |
| 23:DB:1408:G:H2'  | 23:DB:1409:U:C6    | 2.54                     | 0.43              |
| 23:DB:1547:C:H2'  | 23:DB:1548:A:C8    | 2.53                     | 0.43              |
| 23:DB:1987:A:H2'  | 23:DB:1988:G:H8    | 1.82                     | 0.43              |
| 23:DB:2135:A:C6   | 23:DB:2136:G:N7    | 2.87                     | 0.43              |
| 23:DB:2260:C:O2'  | 23:DB:2261:C:H5'   | 2.18                     | 0.43              |
| 23:DB:2581:G:H2'  | 23:DB:2581:G:N3    | 2.34                     | 0.43              |
| 23:DB:2663:G:H2'  | 23:DB:2664:G:C8    | 2.54                     | 0.43              |
| 25:DC:45:ASN:ND2  | 25:DC:50:THR:OG1   | 2.51                     | 0.43              |
| 28:DF:98:PHE:CA   | 28:DF:101:ARG:HE   | 2.23                     | 0.43              |
| 28:DF:133:GLU:HB3 | 28:DF:134:GLN:H    | 1.50                     | 0.43              |
| 29:DG:39:ALA:CA   | 29:DG:54:ARG:HB2   | 2.48                     | 0.43              |
| 29:DG:88:LEU:HG   | 29:DG:161:VAL:HB   | 2.01                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:DL:101:ILE:C   | 33:DL:103:ILE:H    | 2.27                     | 0.43              |
| 34:DM:5:LYS:CE    | 34:DM:6:ARG:H      | 2.23                     | 0.43              |
| 35:DN:100:CYS:SG  | 47:D0:43:THR:HG21  | 2.59                     | 0.43              |
| 36:DO:35:ILE:CG1  | 36:DO:106:LEU:HD12 | 2.47                     | 0.43              |
| 38:DQ:52:ARG:HG2  | 38:DQ:53:LYS:HE2   | 1.99                     | 0.43              |
| 38:DQ:60:TRP:CD2  | 38:DQ:93:ILE:HA    | 2.54                     | 0.43              |
| 38:DQ:78:PHE:C    | 38:DQ:78:PHE:CD1   | 2.97                     | 0.43              |
| 38:DQ:82:LEU:O    | 38:DQ:88:GLU:HG3   | 2.19                     | 0.43              |
| 41:DT:24:MET:HE2  | 41:DT:30:ILE:CA    | 2.49                     | 0.43              |
| 46:DZ:12:ILE:HA   | 46:DZ:26:SER:HA    | 2.01                     | 0.43              |
| 50:D3:41:ARG:HH11 | 50:D3:41:ARG:HG2   | 1.84                     | 0.43              |
| 51:D4:2:LYS:HD3   | 51:D4:2:LYS:H      | 1.84                     | 0.43              |
| 1:AA:223:A:H2'    | 1:AA:224:U:C6      | 2.53                     | 0.43              |
| 1:AA:691:G:H1'    | 1:AA:696:A:H61     | 1.84                     | 0.43              |
| 1:AA:967:C:OP1    | 1:AA:969:A:H8      | 2.00                     | 0.43              |
| 1:AA:1038:C:H2'   | 1:AA:1039:G:C8     | 2.54                     | 0.43              |
| 1:AA:1380:U:O4    | 6:AG:2:ARG:HG3     | 2.18                     | 0.43              |
| 1:AA:1489:G:H2'   | 1:AA:1490:U:C6     | 2.54                     | 0.43              |
| 4:AE:56:PRO:O     | 4:AE:60:GLN:HG3    | 2.19                     | 0.43              |
| 8:AI:94:ARG:CZ    | 8:AI:94:ARG:HB2    | 2.49                     | 0.43              |
| 8:AI:126:PHE:O    | 8:AI:127:SER:C     | 2.62                     | 0.43              |
| 11:AL:64:SER:OG   | 11:AL:96:THR:HG23  | 2.18                     | 0.43              |
| 12:AM:3:ILE:CA    | 12:AM:56:ARG:HG2   | 2.40                     | 0.43              |
| 13:AN:78:LEU:HB2  | 13:AN:83:VAL:HG22  | 1.99                     | 0.43              |
| 17:AR:33:THR:C    | 17:AR:35:SER:H     | 2.26                     | 0.43              |
| 17:AR:62:ARG:HD2  | 17:AR:69:TYR:CD2   | 2.54                     | 0.43              |
| 21:AU:35:GLU:HB2  | 21:AU:37:TYR:CZ    | 2.54                     | 0.43              |
| 23:BB:28:A:O2'    | 23:BB:29:U:H5'     | 2.18                     | 0.43              |
| 23:BB:188:G:OP1   | 46:BZ:11:GLU:HG2   | 2.18                     | 0.43              |
| 23:BB:298:G:C2    | 23:BB:339:U:C5     | 3.06                     | 0.43              |
| 23:BB:1249:U:H4'  | 38:BQ:3:VAL:HG13   | 1.99                     | 0.43              |
| 23:BB:1306:C:H2'  | 23:BB:1307:A:H8    | 1.84                     | 0.43              |
| 23:BB:1399:C:H2'  | 23:BB:1400:U:H6    | 1.84                     | 0.43              |
| 23:BB:1549:A:H2'  | 23:BB:1550:C:H6    | 1.84                     | 0.43              |
| 23:BB:1746:A:H2'  | 23:BB:1747:U:C6    | 2.53                     | 0.43              |
| 23:BB:1857:G:H1'  | 23:BB:1885:A:H62   | 1.82                     | 0.43              |
| 23:BB:1858:A:N6   | 23:BB:1884:G:O2'   | 2.51                     | 0.43              |
| 23:BB:1945:G:C4   | 23:BB:1946:U:C5    | 3.07                     | 0.43              |
| 23:BB:2100:G:C6   | 23:BB:2190:G:C6    | 3.07                     | 0.43              |
| 23:BB:2233:U:H2'  | 23:BB:2234:G:H8    | 1.83                     | 0.43              |
| 23:BB:2660:A:H2'  | 23:BB:2661:G:O4'   | 2.18                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:BB:2691:C:H2'   | 23:BB:2692:G:H8   | 1.83                     | 0.43              |
| 25:BC:51:ARG:HE    | 25:BC:51:ARG:HB2  | 1.61                     | 0.43              |
| 25:BC:66:PHE:HB3   | 25:BC:67:LYS:H    | 1.61                     | 0.43              |
| 26:BD:1:MET:HG3    | 26:BD:205:PRO:HG2 | 2.01                     | 0.43              |
| 26:BD:117:GLY:O    | 26:BD:118:PHE:C   | 2.60                     | 0.43              |
| 28:BF:177:ARG:HH21 | 28:BF:178:LYS:HA  | 1.83                     | 0.43              |
| 29:BG:8:VAL:O      | 29:BG:48:THR:HA   | 2.18                     | 0.43              |
| 30:BH:5:LEU:CD1    | 30:BH:37:VAL:HG11 | 2.48                     | 0.43              |
| 30:BH:30:LEU:HD22  | 30:BH:35:LYS:HE3  | 2.00                     | 0.43              |
| 31:BJ:7:LYS:HZ3    | 31:BJ:49:ASP:N    | 2.12                     | 0.43              |
| 31:BJ:58:ASN:O     | 31:BJ:59:ALA:HB3  | 2.19                     | 0.43              |
| 35:BN:35:LYS:N     | 35:BN:112:TYR:HB3 | 2.33                     | 0.43              |
| 36:BO:1:MET:HG2    | 36:BO:2:ASP:N     | 2.32                     | 0.43              |
| 36:BO:50:ALA:HB1   | 36:BO:79:ALA:HB1  | 2.01                     | 0.43              |
| 41:BT:3:ARG:HE     | 41:BT:8:LEU:HD23  | 1.83                     | 0.43              |
| 41:BT:11:LEU:HD23  | 41:BT:46:ALA:HB1  | 2.00                     | 0.43              |
| 43:BW:76:ARG:HG2   | 43:BW:77:LYS:H    | 1.81                     | 0.43              |
| 1:CA:113:G:H21     | 1:CA:353:A:H8     | 1.66                     | 0.43              |
| 1:CA:186:C:H2'     | 1:CA:187:G:O4'    | 2.18                     | 0.43              |
| 1:CA:709:U:H2'     | 1:CA:710:G:H8     | 1.83                     | 0.43              |
| 1:CA:919:A:O2'     | 1:CA:920:U:H5'    | 2.19                     | 0.43              |
| 1:CA:1013:G:H2'    | 1:CA:1015:G:OP2   | 2.18                     | 0.43              |
| 1:CA:1279:G:N2     | 9:CJ:45:ARG:HD2   | 2.33                     | 0.43              |
| 1:CA:1298:U:H4'    | 1:CA:1299:A:C2    | 2.54                     | 0.43              |
| 1:CA:1314:C:O2'    | 1:CA:1315:U:H5'   | 2.19                     | 0.43              |
| 2:CC:54:ILE:HB     | 2:CC:67:ILE:CD1   | 2.49                     | 0.43              |
| 2:CC:121:SER:O     | 2:CC:125:ARG:HG3  | 2.18                     | 0.43              |
| 2:CC:166:TRP:CG    | 2:CC:167:TYR:H    | 2.37                     | 0.43              |
| 3:CD:24:VAL:O      | 3:CD:25:ARG:C     | 2.62                     | 0.43              |
| 3:CD:106:PHE:HB3   | 3:CD:154:VAL:HG12 | 2.01                     | 0.43              |
| 6:CG:6:ILE:HG22    | 6:CG:7:GLY:N      | 2.34                     | 0.43              |
| 7:CH:21:LYS:O      | 7:CH:62:LEU:HD22  | 2.19                     | 0.43              |
| 12:CM:59:VAL:HG13  | 12:CM:60:ALA:N    | 2.33                     | 0.43              |
| 13:CN:9:GLU:O      | 13:CN:10:VAL:C    | 2.61                     | 0.43              |
| 14:CO:31:LEU:HA    | 14:CO:34:GLN:OE1  | 2.19                     | 0.43              |
| 15:CP:13:LYS:O     | 15:CP:15:PRO:HD3  | 2.18                     | 0.43              |
| 20:CB:216:VAL:C    | 20:CB:218:ALA:H   | 2.26                     | 0.43              |
| 22:DA:14:U:H3'     | 22:DA:15:A:C5'    | 2.48                     | 0.43              |
| 22:DA:14:U:O2'     | 22:DA:107:G:H1'   | 2.19                     | 0.43              |
| 23:DB:282:A:H2'    | 23:DB:283:G:C8    | 2.54                     | 0.43              |
| 23:DB:480:A:C4'    | 42:DU:40:LEU:HD22 | 2.47                     | 0.43              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DB:585:G:N7     | 38:DQ:5:ARG:NH2   | 2.67                     | 0.43              |
| 23:DB:839:U:H2'    | 23:DB:840:C:C6    | 2.53                     | 0.43              |
| 23:DB:1100:C:OP2   | 52:DI:2:LYS:NZ    | 2.38                     | 0.43              |
| 23:DB:1199:U:O2'   | 38:DQ:2:ARG:HB2   | 2.18                     | 0.43              |
| 23:DB:1270:C:H5''  | 23:DB:1271:G:O5'  | 2.19                     | 0.43              |
| 23:DB:1281:G:H2'   | 23:DB:1282:U:O4'  | 2.18                     | 0.43              |
| 23:DB:1559:U:H3'   | 23:DB:1560:G:C5'  | 2.47                     | 0.43              |
| 23:DB:1599:U:C2    | 23:DB:1600:C:C5   | 3.06                     | 0.43              |
| 23:DB:1707:G:H2'   | 23:DB:1708:C:C6   | 2.54                     | 0.43              |
| 23:DB:1858:A:N6    | 23:DB:1884:G:O2'  | 2.51                     | 0.43              |
| 23:DB:1877:A:H2'   | 23:DB:1878:G:C8   | 2.53                     | 0.43              |
| 23:DB:1930:G:C2'   | 23:DB:1931:U:OP2  | 2.67                     | 0.43              |
| 23:DB:1945:G:C4    | 23:DB:1946:U:C5   | 3.07                     | 0.43              |
| 23:DB:2199:A:H3'   | 23:DB:2200:C:H6   | 1.82                     | 0.43              |
| 23:DB:2601:C:C3'   | 23:DB:2602:A:H5'' | 2.47                     | 0.43              |
| 23:DB:2678:C:O2'   | 23:DB:2679:A:H5'  | 2.18                     | 0.43              |
| 24:DV:44:HIS:O     | 24:DV:46:LYS:N    | 2.51                     | 0.43              |
| 25:DC:160:TYR:O    | 25:DC:176:ARG:HG2 | 2.19                     | 0.43              |
| 26:DD:14:ILE:HG23  | 26:DD:19:GLY:CA   | 2.49                     | 0.43              |
| 27:DE:136:GLN:HA   | 27:DE:139:LYS:HG2 | 2.01                     | 0.43              |
| 28:DF:103:ILE:HD12 | 28:DF:104:THR:H   | 1.81                     | 0.43              |
| 29:DG:29:ASN:HB3   | 29:DG:78:VAL:HA   | 2.00                     | 0.43              |
| 31:DJ:41:LYS:HD2   | 31:DJ:44:TYR:C    | 2.43                     | 0.43              |
| 31:DJ:105:VAL:HA   | 31:DJ:108:MET:HE3 | 2.00                     | 0.43              |
| 32:DK:79:PHE:N     | 32:DK:79:PHE:CD1  | 2.86                     | 0.43              |
| 34:DM:14:LYS:HA    | 34:DM:72:PRO:HG3  | 2.00                     | 0.43              |
| 35:DN:80:PHE:O     | 35:DN:85:PRO:HD3  | 2.18                     | 0.43              |
| 35:DN:86:ARG:CZ    | 35:DN:117:ASP:HA  | 2.49                     | 0.43              |
| 40:DS:84:ARG:C     | 40:DS:96:ILE:HG22 | 2.43                     | 0.43              |
| 44:DX:39:GLN:O     | 44:DX:41:HIS:N    | 2.50                     | 0.43              |
| 45:DY:5:LYS:HE2    | 45:DY:58:GLU:OE2  | 2.19                     | 0.43              |
| 48:D1:9:LYS:HA     | 48:D1:24:LYS:HB3  | 2.00                     | 0.43              |
| 49:D2:12:ARG:O     | 49:D2:13:ASN:C    | 2.62                     | 0.43              |
| 1:AA:374:A:H5''    | 1:AA:452:A:N1     | 2.33                     | 0.43              |
| 1:AA:408:A:OP1     | 3:AD:109:THR:HG21 | 2.19                     | 0.43              |
| 1:AA:432:A:C5      | 1:AA:433:G:C8     | 3.07                     | 0.43              |
| 1:AA:448:A:H2'     | 1:AA:449:G:C8     | 2.53                     | 0.43              |
| 1:AA:552:U:H5'     | 11:AL:82:ARG:HH11 | 1.83                     | 0.43              |
| 1:AA:812:G:N3      | 1:AA:812:G:C2'    | 2.77                     | 0.43              |
| 1:AA:995:C:O2      | 1:AA:1047:G:H5'   | 2.18                     | 0.43              |
| 1:AA:1234:C:O2'    | 1:AA:1235:U:H5'   | 2.18                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1292:G:O2'    | 1:AA:1293:C:H5'    | 2.19                     | 0.43              |
| 2:AC:112:ALA:HB2   | 2:AC:182:ASP:O     | 2.19                     | 0.43              |
| 3:AD:84:ASN:OD1    | 4:AE:101:GLY:HA2   | 2.18                     | 0.43              |
| 4:AE:109:ALA:O     | 4:AE:113:VAL:HG13  | 2.19                     | 0.43              |
| 6:AG:110:ARG:HH12  | 6:AG:122:GLU:N     | 2.17                     | 0.43              |
| 7:AH:95:MET:HB3    | 7:AH:99:GLY:H      | 1.84                     | 0.43              |
| 8:AI:51:LEU:HD12   | 8:AI:51:LEU:N      | 2.34                     | 0.43              |
| 9:AJ:93:ALA:HB1    | 9:AJ:96:VAL:CG2    | 2.49                     | 0.43              |
| 10:AK:109:ILE:O    | 10:AK:110:THR:HG23 | 2.18                     | 0.43              |
| 11:AL:41:PRO:HD3   | 11:AL:47:ALA:O     | 2.19                     | 0.43              |
| 21:AU:44:ARG:HG3   | 21:AU:44:ARG:NH1   | 2.32                     | 0.43              |
| 23:BB:281:C:H2'    | 23:BB:282:A:C8     | 2.54                     | 0.43              |
| 23:BB:373:U:O2'    | 23:BB:374:A:H5'    | 2.19                     | 0.43              |
| 23:BB:492:A:H2     | 40:BS:7:HIS:HE1    | 1.67                     | 0.43              |
| 23:BB:502:A:N6     | 23:BB:505:A:N1     | 2.66                     | 0.43              |
| 23:BB:1373:A:H4'   | 23:BB:2212:A:N3    | 2.34                     | 0.43              |
| 23:BB:1426:G:H8    | 23:BB:1426:G:OP2   | 2.01                     | 0.43              |
| 23:BB:2152:G:H2'   | 23:BB:2153:C:C6    | 2.54                     | 0.43              |
| 23:BB:2227:A:O2'   | 25:BC:258:SER:HA   | 2.19                     | 0.43              |
| 23:BB:2247:A:O2'   | 23:BB:2248:C:H5'   | 2.19                     | 0.43              |
| 23:BB:2272:U:C3'   | 23:BB:2272:U:C6    | 3.01                     | 0.43              |
| 23:BB:2450:A:O2'   | 23:BB:2451:A:H5'   | 2.19                     | 0.43              |
| 23:BB:2479:U:OP1   | 51:B4:1:MET:SD     | 2.77                     | 0.43              |
| 23:BB:2511:U:H2'   | 23:BB:2512:C:O4'   | 2.19                     | 0.43              |
| 23:BB:2633:G:H2'   | 23:BB:2634:A:O4'   | 2.19                     | 0.43              |
| 23:BB:2662:A:H2'   | 23:BB:2663:G:O4'   | 2.18                     | 0.43              |
| 25:BC:140:VAL:HG23 | 25:BC:141:HIS:N    | 2.31                     | 0.43              |
| 25:BC:152:GLN:HB3  | 25:BC:153:LEU:HD23 | 2.00                     | 0.43              |
| 25:BC:164:VAL:HG12 | 25:BC:164:VAL:O    | 2.19                     | 0.43              |
| 25:BC:257:ARG:O    | 25:BC:261:ARG:HG3  | 2.18                     | 0.43              |
| 26:BD:8:LYS:CB     | 37:BP:5:LYS:HZ1    | 2.30                     | 0.43              |
| 26:BD:23:PRO:HA    | 26:BD:190:LYS:N    | 2.34                     | 0.43              |
| 26:BD:128:ARG:HH12 | 26:BD:130:GLN:CD   | 2.26                     | 0.43              |
| 27:BE:59:PRO:HD2   | 27:BE:60:TRP:CE2   | 2.54                     | 0.43              |
| 28:BF:55:ASP:OD2   | 28:BF:148:VAL:HG11 | 2.19                     | 0.43              |
| 28:BF:90:LEU:HD12  | 28:BF:90:LEU:N     | 2.34                     | 0.43              |
| 29:BG:121:THR:HG23 | 29:BG:133:LYS:O    | 2.18                     | 0.43              |
| 29:BG:140:ILE:HD12 | 29:BG:141:GLY:N    | 2.34                     | 0.43              |
| 31:BJ:57:LEU:HD12  | 31:BJ:128:ASN:HA   | 2.01                     | 0.43              |
| 32:BK:2:ILE:HG23   | 32:BK:33:ALA:O     | 2.19                     | 0.43              |
| 33:BL:40:SER:O     | 33:BL:41:ARG:HB2   | 2.17                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:BM:50:ARG:HH22  | 34:BM:54:THR:HG21  | 1.83                     | 0.43              |
| 34:BM:131:VAL:O    | 34:BM:132:THR:HB   | 2.18                     | 0.43              |
| 35:BN:29:VAL:HG13  | 35:BN:83:LEU:CD1   | 2.48                     | 0.43              |
| 40:BS:28:LYS:HE3   | 40:BS:29:VAL:N     | 2.34                     | 0.43              |
| 40:BS:89:ALA:CA    | 40:BS:90:LYS:HZ3   | 2.31                     | 0.43              |
| 43:BW:11:ASN:OD1   | 43:BW:12:GLY:N     | 2.52                     | 0.43              |
| 46:BZ:8:LYS:HD2    | 46:BZ:9:TYR:C      | 2.44                     | 0.43              |
| 52:BI:56:VAL:CG2   | 52:BI:68:PHE:HB2   | 2.49                     | 0.43              |
| 1:CA:275:G:O5'     | 16:CQ:15:LYS:HG2   | 2.19                     | 0.43              |
| 1:CA:432:A:C5      | 1:CA:433:G:C8      | 3.07                     | 0.43              |
| 1:CA:607:A:H2'     | 1:CA:608:A:C8      | 2.52                     | 0.43              |
| 1:CA:707:U:H4'     | 10:CK:21:HIS:CD2   | 2.54                     | 0.43              |
| 1:CA:721:G:H4'     | 1:CA:722:G:O4'     | 2.19                     | 0.43              |
| 1:CA:1190:G:OP2    | 2:CC:4:VAL:HB      | 2.19                     | 0.43              |
| 6:CG:100:MET:HA    | 6:CG:103:ILE:HD12  | 2.00                     | 0.43              |
| 7:CH:68:LYS:HA     | 7:CH:68:LYS:HE3    | 2.01                     | 0.43              |
| 12:CM:97:ARG:HB2   | 12:CM:99:GLN:CD    | 2.44                     | 0.43              |
| 13:CN:72:PHE:O     | 13:CN:73:LEU:HG    | 2.18                     | 0.43              |
| 15:CP:8:ARG:CZ     | 15:CP:15:PRO:HB3   | 2.48                     | 0.43              |
| 18:CS:30:LEU:HB3   | 18:CS:48:ILE:HG23  | 2.00                     | 0.43              |
| 23:DB:274:C:H2'    | 23:DB:275:C:C6     | 2.53                     | 0.43              |
| 23:DB:359:G:H2'    | 23:DB:360:U:H5'    | 2.00                     | 0.43              |
| 23:DB:435:C:C2'    | 23:DB:436:C:H5'    | 2.49                     | 0.43              |
| 23:DB:452:G:N2     | 23:DB:458:G:H1'    | 2.33                     | 0.43              |
| 23:DB:565:C:O2'    | 23:DB:566:U:H5'    | 2.18                     | 0.43              |
| 23:DB:693:A:H2'    | 23:DB:694:U:C6     | 2.53                     | 0.43              |
| 23:DB:766:U:H2'    | 23:DB:767:U:H6     | 1.84                     | 0.43              |
| 23:DB:909:A:H2'    | 23:DB:912:C:H5     | 1.83                     | 0.43              |
| 23:DB:1062:G:H2'   | 23:DB:1063:G:H8    | 1.84                     | 0.43              |
| 23:DB:1403:A:H2'   | 23:DB:1404:C:C6    | 2.54                     | 0.43              |
| 23:DB:1426:G:H8    | 23:DB:1426:G:OP2   | 2.02                     | 0.43              |
| 23:DB:1498:C:H2'   | 23:DB:1499:C:C6    | 2.53                     | 0.43              |
| 23:DB:1923:U:H2'   | 23:DB:1924:C:H6    | 1.84                     | 0.43              |
| 23:DB:2728:U:H2'   | 23:DB:2729:G:C8    | 2.53                     | 0.43              |
| 23:DB:2787:C:O2'   | 23:DB:2788:C:H5'   | 2.19                     | 0.43              |
| 23:DB:2821:A:H2'   | 23:DB:2822:G:H8    | 1.82                     | 0.43              |
| 25:DC:21:PRO:HD2   | 25:DC:202:ARG:HH12 | 1.84                     | 0.43              |
| 25:DC:90:ILE:O     | 25:DC:91:ALA:HB3   | 2.19                     | 0.43              |
| 25:DC:104:LEU:HD13 | 25:DC:156:SER:HB2  | 2.01                     | 0.43              |
| 25:DC:155:ARG:HH21 | 25:DC:155:ARG:HG2  | 1.84                     | 0.43              |
| 25:DC:243:PRO:C    | 25:DC:249:VAL:HG23 | 2.43                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 26:DD:42:ASN:O     | 26:DD:43:ASP:CB   | 2.64                     | 0.43              |
| 26:DD:47:ALA:H     | 26:DD:80:TRP:HB2  | 1.83                     | 0.43              |
| 26:DD:60:VAL:HG23  | 26:DD:63:PRO:CD   | 2.48                     | 0.43              |
| 26:DD:128:ARG:O    | 26:DD:129:THR:HB  | 2.19                     | 0.43              |
| 26:DD:173:GLN:HE21 | 26:DD:208:LYS:HB2 | 1.83                     | 0.43              |
| 27:DE:164:LEU:HD22 | 27:DE:164:LEU:C   | 2.44                     | 0.43              |
| 30:DH:69:ALA:O     | 30:DH:73:ASN:N    | 2.52                     | 0.43              |
| 30:DH:70:GLU:C     | 30:DH:72:ILE:H    | 2.27                     | 0.43              |
| 32:DK:4:GLU:O      | 32:DK:5:GLN:HB2   | 2.18                     | 0.43              |
| 32:DK:71:ARG:O     | 32:DK:72:PRO:O    | 2.36                     | 0.43              |
| 33:DL:38:GLN:CD    | 33:DL:39:LYS:HE2  | 2.43                     | 0.43              |
| 35:DN:34:ILE:O     | 35:DN:112:TYR:HD1 | 2.01                     | 0.43              |
| 37:DP:27:VAL:HA    | 37:DP:86:LYS:HB3  | 2.01                     | 0.43              |
| 37:DP:111:GLU:O    | 37:DP:113:LEU:N   | 2.52                     | 0.43              |
| 38:DQ:7:VAL:HG13   | 38:DQ:8:ILE:CD1   | 2.42                     | 0.43              |
| 40:DS:15:GLN:O     | 40:DS:19:LEU:HG   | 2.18                     | 0.43              |
| 43:DW:33:GLY:HA3   | 43:DW:66:VAL:HG21 | 2.01                     | 0.43              |
| 44:DX:31:GLN:HA    | 44:DX:31:GLN:NE2  | 2.29                     | 0.43              |
| 44:DX:55:THR:O     | 44:DX:56:LEU:HB2  | 2.19                     | 0.43              |
| 45:DY:26:LEU:HD21  | 45:DY:46:MET:HG2  | 2.00                     | 0.43              |
| 46:DZ:3:LYS:CE     | 46:DZ:48:GLN:HB2  | 2.49                     | 0.43              |
| 46:DZ:48:GLN:HB3   | 46:DZ:51:VAL:HG23 | 2.01                     | 0.43              |
| 47:D0:32:THR:HG21  | 47:D0:41:HIS:CD2  | 2.53                     | 0.43              |
| 49:D2:19:ARG:HD3   | 49:D2:20:ALA:N    | 2.33                     | 0.43              |
| 51:D4:18:LYS:O     | 51:D4:19:ARG:CB   | 2.67                     | 0.43              |
| 1:AA:167:A:O2'     | 1:AA:168:G:H5'    | 2.19                     | 0.43              |
| 1:AA:233:C:O2'     | 1:AA:234:C:H5'    | 2.19                     | 0.43              |
| 1:AA:513:C:H2'     | 1:AA:514:C:C6     | 2.54                     | 0.43              |
| 1:AA:664:G:H5''    | 17:AR:52:ARG:CZ   | 2.48                     | 0.43              |
| 1:AA:709:U:H2'     | 1:AA:710:G:H8     | 1.84                     | 0.43              |
| 1:AA:1055:A:H4'    | 2:AC:160:GLU:HG3  | 1.99                     | 0.43              |
| 2:AC:72:PRO:HG2    | 2:AC:73:GLY:H     | 1.84                     | 0.43              |
| 2:AC:178:ARG:HG2   | 2:AC:178:ARG:O    | 2.19                     | 0.43              |
| 3:AD:28:ASP:O      | 3:AD:29:THR:OG1   | 2.26                     | 0.43              |
| 3:AD:81:LEU:HD11   | 3:AD:92:LEU:HD21  | 2.00                     | 0.43              |
| 3:AD:117:VAL:HG12  | 3:AD:130:ASN:HA   | 2.01                     | 0.43              |
| 7:AH:17:GLN:OE1    | 7:AH:69:ALA:HB1   | 2.19                     | 0.43              |
| 9:AJ:89:ARG:O      | 9:AJ:90:LEU:HD23  | 2.19                     | 0.43              |
| 11:AL:56:LEU:HD11  | 11:AL:81:ILE:CD1  | 2.41                     | 0.43              |
| 14:AO:2:LEU:HD22   | 14:AO:7:THR:HG23  | 2.00                     | 0.43              |
| 16:AQ:60:ILE:HB    | 16:AQ:72:TRP:CE3  | 2.54                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:AB:121:GLN:HB3  | 20:AB:121:GLN:HE21 | 1.52                     | 0.43              |
| 23:BB:36:G:H4'     | 23:BB:451:U:N3     | 2.34                     | 0.43              |
| 23:BB:100:U:H2'    | 23:BB:100:U:OP1    | 2.18                     | 0.43              |
| 23:BB:357:C:H2'    | 23:BB:358:U:C6     | 2.54                     | 0.43              |
| 23:BB:756:A:H2'    | 23:BB:757:G:O4'    | 2.19                     | 0.43              |
| 23:BB:1076:C:O2'   | 23:BB:1077:A:H5'   | 2.19                     | 0.43              |
| 23:BB:1081:U:O2'   | 23:BB:1082:U:H5'   | 2.19                     | 0.43              |
| 23:BB:1281:G:H2'   | 23:BB:1282:U:O4'   | 2.18                     | 0.43              |
| 23:BB:1704:C:H2'   | 23:BB:1705:A:C8    | 2.54                     | 0.43              |
| 23:BB:1707:G:H2'   | 23:BB:1708:C:C6    | 2.54                     | 0.43              |
| 25:BC:75:ALA:HB1   | 25:BC:93:VAL:HG13  | 2.01                     | 0.43              |
| 25:BC:153:LEU:O    | 25:BC:153:LEU:HG   | 2.19                     | 0.43              |
| 26:BD:154:LYS:C    | 26:BD:156:PHE:N    | 2.62                     | 0.43              |
| 27:BE:25:GLU:OE2   | 33:BL:16:GLY:HA2   | 2.19                     | 0.43              |
| 27:BE:105:LEU:C    | 27:BE:107:SER:H    | 2.26                     | 0.43              |
| 27:BE:145:ASP:C    | 27:BE:147:LEU:N    | 2.71                     | 0.43              |
| 27:BE:153:LEU:HD11 | 27:BE:201:ALA:HA   | 2.00                     | 0.43              |
| 28:BF:2:LYS:HE2    | 28:BF:2:LYS:CA     | 2.48                     | 0.43              |
| 29:BG:137:LYS:HA   | 29:BG:140:ILE:HG13 | 2.00                     | 0.43              |
| 30:BH:28:ASN:HA    | 30:BH:32:PRO:HG3   | 2.00                     | 0.43              |
| 30:BH:89:LYS:NZ    | 30:BH:123:ARG:HD3  | 2.34                     | 0.43              |
| 32:BK:113:MET:HE1  | 32:BK:116:ILE:HD11 | 2.01                     | 0.43              |
| 33:BL:60:ARG:HD3   | 50:B3:11:LYS:CE    | 2.49                     | 0.43              |
| 34:BM:36:VAL:HG21  | 34:BM:125:PRO:HD3  | 2.00                     | 0.43              |
| 34:BM:43:ALA:HB2   | 34:BM:91:TYR:O     | 2.18                     | 0.43              |
| 35:BN:57:THR:CB    | 35:BN:61:ALA:HB3   | 2.49                     | 0.43              |
| 38:BQ:33:VAL:O     | 38:BQ:36:GLN:N     | 2.50                     | 0.43              |
| 38:BQ:35:PHE:HA    | 38:BQ:39:ILE:HD12  | 2.00                     | 0.43              |
| 38:BQ:102:LYS:H    | 38:BQ:102:LYS:CD   | 2.29                     | 0.43              |
| 42:BU:78:LYS:CG    | 42:BU:96:LYS:HE3   | 2.48                     | 0.43              |
| 44:BX:24:GLU:O     | 44:BX:25:GLN:C     | 2.62                     | 0.43              |
| 46:BZ:3:LYS:HA     | 46:BZ:47:LYS:HA    | 2.00                     | 0.43              |
| 47:B0:11:LYS:C     | 47:B0:13:GLY:N     | 2.77                     | 0.43              |
| 47:B0:43:THR:O     | 47:B0:44:ALA:C     | 2.62                     | 0.43              |
| 1:CA:513:C:H2'     | 1:CA:514:C:C6      | 2.53                     | 0.43              |
| 1:CA:730:G:O6      | 14:CO:50:HIS:NE2   | 2.49                     | 0.43              |
| 1:CA:822:U:O2'     | 1:CA:823:C:H5'     | 2.19                     | 0.43              |
| 1:CA:979:C:H41     | 1:CA:1360:A:H62    | 1.67                     | 0.43              |
| 1:CA:1067:A:H3'    | 1:CA:1094:G:OP1    | 2.19                     | 0.43              |
| 1:CA:1409:C:O2     | 23:DB:1913:A:N6    | 2.52                     | 0.43              |
| 3:CD:44:LYS:NZ     | 3:CD:46:ARG:HA     | 2.34                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 10:CK:63:GLN:HG3   | 10:CK:98:ALA:HB2  | 2.01                     | 0.43              |
| 12:CM:37:GLY:O     | 12:CM:38:ILE:HD13 | 2.18                     | 0.43              |
| 20:CB:216:VAL:HG23 | 20:CB:217:ALA:N   | 2.34                     | 0.43              |
| 22:DA:32:U:C2      | 22:DA:33:G:C8     | 3.07                     | 0.43              |
| 23:DB:593:U:H2'    | 23:DB:594:U:H6    | 1.81                     | 0.43              |
| 23:DB:598:U:C5'    | 33:DL:21:ARG:HB2  | 2.45                     | 0.43              |
| 23:DB:878:A:H1'    | 23:DB:899:A:H62   | 1.83                     | 0.43              |
| 23:DB:1704:C:H2'   | 23:DB:1705:A:C8   | 2.54                     | 0.43              |
| 23:DB:1829:A:H3'   | 23:DB:1830:C:H6   | 1.84                     | 0.43              |
| 23:DB:2157:G:N3    | 23:DB:2157:G:C2'  | 2.79                     | 0.43              |
| 23:DB:2361:G:O2'   | 23:DB:2362:C:H5'  | 2.18                     | 0.43              |
| 23:DB:2466:C:O2'   | 23:DB:2467:C:H5'  | 2.17                     | 0.43              |
| 23:DB:2564:A:OP1   | 23:DB:2648:G:H4'  | 2.18                     | 0.43              |
| 27:DE:176:ASP:OD1  | 27:DE:177:PRO:HD2 | 2.19                     | 0.43              |
| 29:DG:8:VAL:CG1    | 29:DG:49:LEU:HD12 | 2.48                     | 0.43              |
| 32:DK:10:VAL:HG21  | 32:DK:17:ARG:N    | 2.34                     | 0.43              |
| 33:DL:107:PHE:HE2  | 33:DL:126:ARG:HB2 | 1.84                     | 0.43              |
| 34:DM:17:ASN:O     | 34:DM:17:ASN:CG   | 2.61                     | 0.43              |
| 34:DM:73:ILE:CD1   | 34:DM:92:TRP:HE3  | 2.32                     | 0.43              |
| 34:DM:106:ASP:C    | 34:DM:109:PRO:HD3 | 2.44                     | 0.43              |
| 38:DQ:25:GLY:O     | 38:DQ:29:ARG:HG3  | 2.18                     | 0.43              |
| 38:DQ:40:LYS:HB2   | 38:DQ:40:LYS:HZ3  | 1.82                     | 0.43              |
| 39:DR:18:GLN:HB3   | 39:DR:99:THR:HB   | 2.01                     | 0.43              |
| 39:DR:68:ARG:H     | 39:DR:97:LYS:HG3  | 1.84                     | 0.43              |
| 40:DS:45:VAL:C     | 40:DS:47:VAL:N    | 2.77                     | 0.43              |
| 42:DU:46:LYS:HG2   | 42:DU:53:GLN:HB2  | 2.01                     | 0.43              |
| 44:DX:17:GLU:CA    | 44:DX:21:LEU:HB2  | 2.49                     | 0.43              |
| 45:DY:35:VAL:HG12  | 45:DY:36:GLU:H    | 1.83                     | 0.43              |
| 46:DZ:27:THR:C     | 46:DZ:28:VAL:HG22 | 2.44                     | 0.43              |
| 46:DZ:49:ARG:O     | 46:DZ:52:ALA:N    | 2.50                     | 0.43              |
| 47:D0:46:GLY:O     | 47:D0:47:TYR:HB3  | 2.18                     | 0.43              |
| 50:D3:39:ARG:HD3   | 50:D3:39:ARG:HA   | 1.76                     | 0.43              |
| 52:DI:54:ILE:HD11  | 52:DI:71:LYS:O    | 2.19                     | 0.43              |
| 1:AA:25:C:H2'      | 1:AA:26:A:C8      | 2.54                     | 0.43              |
| 1:AA:155:A:H2'     | 1:AA:156:C:O4'    | 2.19                     | 0.43              |
| 1:AA:371:A:H2'     | 1:AA:372:C:C6     | 2.54                     | 0.43              |
| 1:AA:401:C:O2'     | 1:AA:402:G:H5'    | 2.18                     | 0.43              |
| 1:AA:484:G:O2'     | 1:AA:485:U:OP2    | 2.29                     | 0.43              |
| 1:AA:529:G:H22     | 11:AL:47:ALA:HB3  | 1.84                     | 0.43              |
| 1:AA:626:G:H2'     | 1:AA:627:G:H8     | 1.83                     | 0.43              |
| 1:AA:659:U:O2'     | 1:AA:660:C:H5'    | 2.18                     | 0.43              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:721:G:H4'     | 1:AA:722:G:O4'     | 2.19                     | 0.43              |
| 1:AA:861:G:H2'     | 1:AA:862:C:H6      | 1.84                     | 0.43              |
| 1:AA:1263:C:H2'    | 1:AA:1264:U:H6     | 1.84                     | 0.43              |
| 1:AA:1322:C:O2     | 1:AA:1322:C:O4'    | 2.37                     | 0.43              |
| 5:AF:7:VAL:HG23    | 5:AF:60:VAL:O      | 2.18                     | 0.43              |
| 8:AI:82:ILE:HG22   | 8:AI:86:LEU:HD21   | 2.01                     | 0.43              |
| 9:AJ:7:ARG:HG2     | 9:AJ:75:ASP:OD2    | 2.18                     | 0.43              |
| 9:AJ:57:VAL:HG13   | 9:AJ:58:ASN:N      | 2.33                     | 0.43              |
| 16:AQ:10:ARG:HH22  | 16:AQ:58:VAL:HG13  | 1.84                     | 0.43              |
| 20:AB:217:ALA:O    | 20:AB:221:ARG:HG3  | 2.18                     | 0.43              |
| 23:BB:285:G:C2'    | 23:BB:286:U:H5'    | 2.49                     | 0.43              |
| 23:BB:511:U:O5'    | 23:BB:511:U:H6     | 2.01                     | 0.43              |
| 23:BB:832:U:OP1    | 33:BL:45:GLY:N     | 2.46                     | 0.43              |
| 23:BB:848:C:H3'    | 23:BB:849:A:H8     | 1.83                     | 0.43              |
| 23:BB:971:G:H2'    | 23:BB:972:A:O4'    | 2.19                     | 0.43              |
| 23:BB:975:A:H1'    | 23:BB:990:A:C2     | 2.54                     | 0.43              |
| 23:BB:1244:A:H4'   | 33:BL:15:ALA:HB1   | 2.00                     | 0.43              |
| 23:BB:1359:A:H2'   | 23:BB:1360:G:O4'   | 2.17                     | 0.43              |
| 23:BB:1634:A:H3'   | 23:BB:1635:A:C5'   | 2.48                     | 0.43              |
| 23:BB:1773:A:H2'   | 23:BB:1774:C:O4'   | 2.19                     | 0.43              |
| 23:BB:2061:G:H8    | 23:BB:2501:C:HO2'  | 1.62                     | 0.43              |
| 23:BB:2330:G:O2'   | 43:BW:36:ILE:HD11  | 2.18                     | 0.43              |
| 23:BB:2511:U:O5'   | 23:BB:2511:U:H6    | 2.02                     | 0.43              |
| 23:BB:2574:G:HO2'  | 26:BD:151:THR:HG21 | 1.84                     | 0.43              |
| 23:BB:2663:G:H2'   | 23:BB:2664:G:C8    | 2.54                     | 0.43              |
| 23:BB:2671:G:O2'   | 23:BB:2672:U:H5'   | 2.19                     | 0.43              |
| 23:BB:2811:G:H2'   | 23:BB:2812:G:H8    | 1.83                     | 0.43              |
| 24:BV:77:VAL:HG12  | 34:BM:133:LYS:HZ2  | 1.84                     | 0.43              |
| 25:BC:224:MET:HE3  | 25:BC:232:GLY:CA   | 2.49                     | 0.43              |
| 25:BC:225:ASN:HD22 | 25:BC:225:ASN:HA   | 1.52                     | 0.43              |
| 25:BC:247:TRP:HD1  | 25:BC:247:TRP:O    | 2.02                     | 0.43              |
| 27:BE:144:GLU:HG3  | 27:BE:145:ASP:N    | 2.34                     | 0.43              |
| 27:BE:189:THR:O    | 27:BE:190:ALA:HB3  | 2.19                     | 0.43              |
| 31:BJ:80:HIS:HB2   | 31:BJ:84:ILE:HD11  | 1.99                     | 0.43              |
| 32:BK:108:ARG:HG3  | 32:BK:108:ARG:HH11 | 1.83                     | 0.43              |
| 33:BL:61:LEU:CB    | 33:BL:62:PRO:CD    | 2.92                     | 0.43              |
| 34:BM:107:GLY:C    | 34:BM:109:PRO:HD3  | 2.44                     | 0.43              |
| 35:BN:99:LYS:NZ    | 35:BN:99:LYS:CB    | 2.79                     | 0.43              |
| 36:BO:67:ASN:HA    | 36:BO:67:ASN:HD22  | 1.65                     | 0.43              |
| 37:BP:51:ASN:HA    | 37:BP:60:VAL:HB    | 2.00                     | 0.43              |
| 40:BS:29:VAL:H     | 40:BS:71:VAL:HG21  | 1.84                     | 0.43              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:BS:33:LEU:O    | 40:BS:35:ILE:N     | 2.50                     | 0.43              |
| 44:BX:18:LEU:HD23 | 44:BX:18:LEU:N     | 2.34                     | 0.43              |
| 49:B2:3:ARG:HB3   | 49:B2:5:PHE:HE1    | 1.84                     | 0.43              |
| 50:B3:22:LYS:HD2  | 50:B3:46:LYS:HA    | 1.99                     | 0.43              |
| 52:BI:75:ALA:CB   | 52:BI:131:THR:HG21 | 2.49                     | 0.43              |
| 1:CA:113:G:C1'    | 1:CA:354:G:H5'     | 2.49                     | 0.43              |
| 1:CA:179:A:H2'    | 1:CA:180:U:C6      | 2.54                     | 0.43              |
| 1:CA:408:A:H3'    | 1:CA:409:U:C6      | 2.47                     | 0.43              |
| 1:CA:453:G:C6     | 1:CA:454:G:C6      | 3.06                     | 0.43              |
| 1:CA:635:A:H2'    | 1:CA:636:U:C6      | 2.53                     | 0.43              |
| 1:CA:814:A:H5'    | 1:CA:1511:G:C4'    | 2.42                     | 0.43              |
| 1:CA:815:A:N6     | 1:CA:1509:C:H1'    | 2.32                     | 0.43              |
| 1:CA:1309:G:H5'   | 12:CM:76:ILE:HG12  | 2.00                     | 0.43              |
| 2:CC:166:TRP:HE1  | 2:CC:168:ARG:CB    | 2.32                     | 0.43              |
| 5:CF:97:THR:C     | 5:CF:98:GLU:HG2    | 2.44                     | 0.43              |
| 6:CG:29:LEU:CD2   | 6:CG:104:VAL:HG13  | 2.49                     | 0.43              |
| 7:CH:50:VAL:HG23  | 7:CH:57:GLU:O      | 2.19                     | 0.43              |
| 12:CM:6:ILE:O     | 12:CM:7:ASN:C      | 2.62                     | 0.43              |
| 13:CN:26:LEU:O    | 13:CN:44:VAL:HG11  | 2.19                     | 0.43              |
| 15:CP:44:SER:C    | 15:CP:46:LYS:N     | 2.73                     | 0.43              |
| 16:CQ:35:LYS:O    | 16:CQ:37:ILE:HG23  | 2.19                     | 0.43              |
| 20:CB:111:LYS:O   | 20:CB:114:LYS:HB3  | 2.19                     | 0.43              |
| 22:DA:111:U:O2'   | 22:DA:112:G:H5'    | 2.18                     | 0.43              |
| 23:DB:539:G:H2'   | 23:DB:540:C:C6     | 2.54                     | 0.43              |
| 23:DB:630:G:N1    | 33:DL:69:ARG:NH1   | 2.66                     | 0.43              |
| 23:DB:981:A:N1    | 23:DB:2027:G:O2'   | 2.43                     | 0.43              |
| 23:DB:1841:U:C2   | 23:DB:1842:G:C8    | 3.07                     | 0.43              |
| 23:DB:1891:G:H2'  | 23:DB:1892:C:H6    | 1.84                     | 0.43              |
| 23:DB:2256:G:H2'  | 23:DB:2257:U:H6    | 1.84                     | 0.43              |
| 23:DB:2341:G:H2'  | 23:DB:2342:C:C6    | 2.54                     | 0.43              |
| 23:DB:2405:G:H5'  | 33:DL:70:LYS:CG    | 2.49                     | 0.43              |
| 23:DB:2450:A:O2'  | 23:DB:2451:A:H5'   | 2.19                     | 0.43              |
| 23:DB:2782:G:O2'  | 23:DB:2783:U:H5'   | 2.19                     | 0.43              |
| 25:DC:106:PRO:HB2 | 25:DC:107:LYS:H    | 1.68                     | 0.43              |
| 25:DC:235:GLU:CG  | 25:DC:236:GLY:H    | 2.30                     | 0.43              |
| 26:DD:4:LEU:HB3   | 26:DD:202:ILE:HA   | 2.01                     | 0.43              |
| 26:DD:25:THR:HG22 | 26:DD:188:LEU:CD1  | 2.49                     | 0.43              |
| 26:DD:172:VAL:HB  | 26:DD:175:LEU:HD11 | 2.00                     | 0.43              |
| 26:DD:191:GLY:O   | 26:DD:192:ALA:HB3  | 2.17                     | 0.43              |
| 27:DE:137:LYS:C   | 27:DE:138:LEU:HD23 | 2.44                     | 0.43              |
| 28:DF:16:MET:HE1  | 28:DF:22:ASN:N     | 2.34                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:DH:4:ILE:CD1   | 30:DH:37:VAL:HG13 | 2.49                     | 0.43              |
| 33:DL:79:LEU:H    | 33:DL:113:ALA:CB  | 2.31                     | 0.43              |
| 34:DM:133:LYS:CD  | 34:DM:134:THR:H   | 2.30                     | 0.43              |
| 35:DN:4:ARG:CZ    | 35:DN:4:ARG:HB3   | 2.49                     | 0.43              |
| 35:DN:21:PHE:HA   | 35:DN:24:MET:HB3  | 2.01                     | 0.43              |
| 36:DO:94:ARG:O    | 36:DO:95:SER:C    | 2.62                     | 0.43              |
| 37:DP:20:ARG:HH21 | 37:DP:20:ARG:HG2  | 1.84                     | 0.43              |
| 39:DR:38:VAL:O    | 39:DR:41:ILE:HG22 | 2.18                     | 0.43              |
| 39:DR:76:LYS:HE3  | 39:DR:90:ARG:HD3  | 2.01                     | 0.43              |
| 41:DT:47:VAL:CG2  | 41:DT:53:VAL:HG21 | 2.42                     | 0.43              |
| 43:DW:17:ALA:O    | 43:DW:18:LYS:CG   | 2.66                     | 0.43              |
| 46:DZ:3:LYS:HE2   | 46:DZ:48:GLN:HB2  | 2.00                     | 0.43              |
| 48:D1:15:GLY:O    | 48:D1:16:THR:C    | 2.61                     | 0.43              |
| 51:D4:19:ARG:HB3  | 51:D4:20:ASP:H    | 1.47                     | 0.43              |
| 1:AA:113:G:C1'    | 1:AA:354:G:H5'    | 2.49                     | 0.42              |
| 1:AA:179:A:H2'    | 1:AA:180:U:H6     | 1.83                     | 0.42              |
| 1:AA:208:U:H2'    | 1:AA:210:C:C5     | 2.54                     | 0.42              |
| 1:AA:332:G:P      | 19:AT:2:ASN:HB3   | 2.59                     | 0.42              |
| 1:AA:349:A:H2'    | 1:AA:350:G:C8     | 2.54                     | 0.42              |
| 1:AA:538:G:H2'    | 1:AA:539:A:C8     | 2.54                     | 0.42              |
| 1:AA:997:U:H2'    | 1:AA:998:C:H6     | 1.82                     | 0.42              |
| 1:AA:1035:A:C2'   | 1:AA:1036:A:H8    | 2.27                     | 0.42              |
| 1:AA:1072:G:H2'   | 1:AA:1073:U:O4'   | 2.19                     | 0.42              |
| 3:AD:138:PRO:HA   | 3:AD:181:PHE:HD2  | 1.83                     | 0.42              |
| 3:AD:201:GLU:CG   | 4:AE:103:GLY:HA3  | 2.49                     | 0.42              |
| 4:AE:145:ASN:O    | 4:AE:146:MET:C    | 2.62                     | 0.42              |
| 6:AG:115:MET:CE   | 6:AG:119:LEU:HB2  | 2.47                     | 0.42              |
| 8:AI:115:VAL:HG23 | 9:AJ:62:ARG:HD2   | 2.00                     | 0.42              |
| 11:AL:58:ASN:H    | 11:AL:58:ASN:HD22 | 1.66                     | 0.42              |
| 11:AL:106:VAL:CG2 | 11:AL:109:ARG:HG3 | 2.48                     | 0.42              |
| 12:AM:77:LYS:HD3  | 12:AM:77:LYS:C    | 2.44                     | 0.42              |
| 14:AO:71:ARG:HH11 | 14:AO:71:ARG:CB   | 2.32                     | 0.42              |
| 18:AS:29:PRO:HB3  | 18:AS:47:THR:HB   | 2.00                     | 0.42              |
| 19:AT:4:LYS:HD2   | 19:AT:5:SER:H     | 1.82                     | 0.42              |
| 19:AT:50:PHE:CE2  | 19:AT:75:LYS:HA   | 2.53                     | 0.42              |
| 20:AB:21:TYR:O    | 20:AB:22:TRP:O    | 2.36                     | 0.42              |
| 20:AB:37:VAL:CG2  | 20:AB:38:HIS:N    | 2.81                     | 0.42              |
| 23:BB:241:A:H4'   | 50:B3:63:TYR:OH   | 2.18                     | 0.42              |
| 23:BB:402:A:C2'   | 23:BB:403:U:H5'   | 2.49                     | 0.42              |
| 23:BB:995:C:C4    | 31:BJ:2:LYS:HB3   | 2.54                     | 0.42              |
| 23:BB:1062:G:H2'  | 23:BB:1063:G:H8   | 1.84                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:1079:C:C2   | 23:BB:1080:A:C8    | 3.07                     | 0.42              |
| 23:BB:1314:C:O2   | 23:BB:1314:C:H2'   | 2.18                     | 0.42              |
| 23:BB:1526:C:O2'  | 23:BB:1527:G:H5'   | 2.19                     | 0.42              |
| 23:BB:1917:U:H2'  | 23:BB:1918:A:C5'   | 2.48                     | 0.42              |
| 23:BB:2052:A:C4   | 26:BD:155:VAL:HG23 | 2.54                     | 0.42              |
| 23:BB:2270:A:C5'  | 43:BW:18:LYS:HB3   | 2.49                     | 0.42              |
| 23:BB:2290:G:H2'  | 23:BB:2291:U:C6    | 2.53                     | 0.42              |
| 23:BB:2333:A:O2'  | 36:BO:7:ARG:HD3    | 2.19                     | 0.42              |
| 25:BC:78:GLU:CB   | 25:BC:92:LEU:HD23  | 2.49                     | 0.42              |
| 25:BC:198:GLU:HA  | 25:BC:201:LEU:HB2  | 2.01                     | 0.42              |
| 26:BD:108:ASP:CB  | 26:BD:173:GLN:HA   | 2.48                     | 0.42              |
| 26:BD:130:GLN:O   | 26:BD:140:HIS:ND1  | 2.51                     | 0.42              |
| 26:BD:165:MET:CE  | 26:BD:166:GLY:H    | 2.31                     | 0.42              |
| 27:BE:128:ALA:CA  | 27:BE:157:LEU:HD22 | 2.48                     | 0.42              |
| 28:BF:15:LEU:O    | 28:BF:18:GLU:O     | 2.37                     | 0.42              |
| 28:BF:67:THR:OG1  | 28:BF:85:GLY:HA3   | 2.19                     | 0.42              |
| 29:BG:5:LYS:O     | 29:BG:68:ARG:NH1   | 2.52                     | 0.42              |
| 31:BJ:7:LYS:HD2   | 31:BJ:49:ASP:CB    | 2.44                     | 0.42              |
| 31:BJ:102:GLU:CG  | 31:BJ:124:VAL:HG11 | 2.49                     | 0.42              |
| 32:BK:71:ARG:HD3  | 32:BK:71:ARG:HA    | 1.87                     | 0.42              |
| 33:BL:38:GLN:HA   | 33:BL:41:ARG:NH1   | 2.34                     | 0.42              |
| 34:BM:134:THR:O   | 34:BM:135:VAL:HG13 | 2.18                     | 0.42              |
| 40:BS:14:ALA:O    | 40:BS:15:GLN:C     | 2.62                     | 0.42              |
| 41:BT:47:VAL:HB   | 41:BT:55:VAL:HG21  | 2.00                     | 0.42              |
| 41:BT:50:LEU:O    | 41:BT:51:PHE:HB2   | 2.18                     | 0.42              |
| 43:BW:35:ILE:CG2  | 43:BW:36:ILE:H     | 2.14                     | 0.42              |
| 47:B0:53:VAL:HG12 | 47:B0:54:ILE:N     | 2.34                     | 0.42              |
| 48:B1:47:ILE:HG13 | 48:B1:48:TYR:N     | 2.34                     | 0.42              |
| 48:B1:53:ILE:CD1  | 48:B1:54:LYS:H     | 2.32                     | 0.42              |
| 1:CA:69:G:N2      | 1:CA:71:A:H62      | 2.16                     | 0.42              |
| 1:CA:179:A:H2'    | 1:CA:180:U:H6      | 1.84                     | 0.42              |
| 1:CA:406:G:H21    | 3:CD:115:GLN:HE22  | 1.65                     | 0.42              |
| 1:CA:697:U:C2'    | 1:CA:698:G:H5'     | 2.49                     | 0.42              |
| 1:CA:861:G:H2'    | 1:CA:862:C:H6      | 1.84                     | 0.42              |
| 1:CA:975:A:H1'    | 1:CA:1358:U:O2     | 2.19                     | 0.42              |
| 1:CA:994:A:N3     | 1:CA:994:A:H2'     | 2.34                     | 0.42              |
| 1:CA:1264:U:H2'   | 1:CA:1265:C:O4'    | 2.19                     | 0.42              |
| 1:CA:1521:C:H2'   | 1:CA:1522:U:H6     | 1.83                     | 0.42              |
| 2:CC:168:ARG:HE   | 2:CC:169:GLU:N     | 2.17                     | 0.42              |
| 3:CD:170:LEU:CA   | 3:CD:182:LYS:HG3   | 2.48                     | 0.42              |
| 5:CF:3:HIS:CB     | 5:CF:92:THR:HA     | 2.31                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:CI:21:LYS:O     | 8:CI:61:ASP:N      | 2.51                     | 0.42              |
| 9:CJ:8:ILE:HG12   | 9:CJ:75:ASP:HA     | 2.00                     | 0.42              |
| 9:CJ:9:ARG:HA     | 9:CJ:9:ARG:HH11    | 1.84                     | 0.42              |
| 9:CJ:40:ILE:HG12  | 9:CJ:74:VAL:H      | 1.84                     | 0.42              |
| 13:CN:13:VAL:HA   | 13:CN:59:GLN:HE21  | 1.84                     | 0.42              |
| 13:CN:50:LEU:HD12 | 13:CN:51:PRO:CD    | 2.46                     | 0.42              |
| 17:CR:20:ILE:O    | 17:CR:20:ILE:HG23  | 2.19                     | 0.42              |
| 20:CB:121:GLN:NE2 | 20:CB:122:ASP:N    | 2.67                     | 0.42              |
| 22:DA:60:C:H2'    | 22:DA:61:G:H8      | 1.83                     | 0.42              |
| 23:DB:153:U:O5'   | 23:DB:153:U:H6     | 2.02                     | 0.42              |
| 23:DB:409:G:O2'   | 23:DB:410:G:H5'    | 2.19                     | 0.42              |
| 23:DB:758:C:O2    | 23:DB:1981:A:H2    | 2.01                     | 0.42              |
| 23:DB:818:G:H4'   | 23:DB:838:C:O3'    | 2.19                     | 0.42              |
| 23:DB:1513:U:O2'  | 23:DB:1514:G:H5'   | 2.19                     | 0.42              |
| 23:DB:1770:G:O2'  | 23:DB:1771:C:H5'   | 2.19                     | 0.42              |
| 23:DB:1803:A:H2   | 23:DB:1823:G:O4'   | 2.02                     | 0.42              |
| 23:DB:1998:A:H2'  | 23:DB:1999:C:H6    | 1.84                     | 0.42              |
| 23:DB:2076:U:OP2  | 23:DB:2238:G:N2    | 2.48                     | 0.42              |
| 23:DB:2094:A:H5'' | 30:DH:22:LYS:HG3   | 2.01                     | 0.42              |
| 23:DB:2294:G:P    | 36:DO:9:ARG:NE     | 2.92                     | 0.42              |
| 23:DB:2336:A:HO2' | 23:DB:2337:G:P     | 2.41                     | 0.42              |
| 23:DB:2385:C:H2'  | 23:DB:2386:A:C8    | 2.53                     | 0.42              |
| 23:DB:2428:G:H5'' | 23:DB:2429:G:O5'   | 2.18                     | 0.42              |
| 23:DB:2511:U:H2'  | 23:DB:2512:C:O4'   | 2.19                     | 0.42              |
| 23:DB:2513:A:H2'  | 23:DB:2514:U:C6    | 2.54                     | 0.42              |
| 23:DB:2671:G:H2'  | 23:DB:2672:U:H6    | 1.80                     | 0.42              |
| 23:DB:2811:G:H2'  | 23:DB:2812:G:C8    | 2.54                     | 0.42              |
| 23:DB:2813:A:O2'  | 23:DB:2814:A:H5'   | 2.18                     | 0.42              |
| 24:DV:44:HIS:C    | 24:DV:46:LYS:N     | 2.77                     | 0.42              |
| 25:DC:50:THR:C    | 25:DC:51:ARG:HG3   | 2.43                     | 0.42              |
| 25:DC:172:THR:HB  | 25:DC:173:LEU:H    | 1.56                     | 0.42              |
| 26:DD:11:MET:O    | 26:DD:22:ILE:HD12  | 2.19                     | 0.42              |
| 26:DD:109:VAL:HA  | 26:DD:203:VAL:HA   | 2.01                     | 0.42              |
| 26:DD:113:SER:O   | 26:DD:167:ASN:HB2  | 2.19                     | 0.42              |
| 28:DF:41:GLU:N    | 28:DF:41:GLU:OE1   | 2.52                     | 0.42              |
| 29:DG:17:LYS:HE3  | 29:DG:17:LYS:C     | 2.44                     | 0.42              |
| 30:DH:12:LEU:HD22 | 30:DH:19:VAL:CG1   | 2.49                     | 0.42              |
| 30:DH:77:THR:HG22 | 30:DH:143:ILE:HB   | 2.00                     | 0.42              |
| 31:DJ:62:VAL:HG11 | 31:DJ:101:ILE:HD11 | 2.00                     | 0.42              |
| 36:DO:71:ALA:O    | 36:DO:74:VAL:HG22  | 2.19                     | 0.42              |
| 37:DP:32:VAL:O    | 37:DP:34:GLY:N     | 2.51                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:DQ:32:ARG:NH1  | 38:DQ:32:ARG:HG2  | 2.32                     | 0.42              |
| 39:DR:67:GLY:H    | 39:DR:98:ILE:N    | 2.17                     | 0.42              |
| 39:DR:69:GLY:HA3  | 39:DR:96:VAL:HG13 | 2.00                     | 0.42              |
| 40:DS:23:LEU:CB   | 47:D0:21:LEU:HD13 | 2.37                     | 0.42              |
| 41:DT:34:VAL:O    | 41:DT:81:LYS:HB3  | 2.19                     | 0.42              |
| 43:DW:36:ILE:HG13 | 43:DW:37:VAL:N    | 2.34                     | 0.42              |
| 45:DY:5:LYS:HB2   | 45:DY:5:LYS:NZ    | 2.34                     | 0.42              |
| 45:DY:5:LYS:O     | 45:DY:56:VAL:HG12 | 2.19                     | 0.42              |
| 48:D1:24:LYS:HD3  | 48:D1:24:LYS:O    | 2.19                     | 0.42              |
| 52:DI:49:GLU:HB2  | 52:DI:52:LEU:HD12 | 2.00                     | 0.42              |
| 1:AA:93:U:H2'     | 1:AA:95:C:H5      | 1.83                     | 0.42              |
| 1:AA:113:G:O4'    | 1:AA:354:G:H4'    | 2.19                     | 0.42              |
| 1:AA:425:G:O2'    | 1:AA:426:U:H5'    | 2.18                     | 0.42              |
| 1:AA:523:A:H61    | 11:AL:88:ASP:HB2  | 1.84                     | 0.42              |
| 1:AA:644:U:O2'    | 1:AA:645:G:H5'    | 2.20                     | 0.42              |
| 1:AA:697:U:C2'    | 1:AA:698:G:H5'    | 2.49                     | 0.42              |
| 1:AA:738:C:H2'    | 1:AA:739:C:C6     | 2.55                     | 0.42              |
| 1:AA:822:U:O2'    | 1:AA:823:C:H5'    | 2.19                     | 0.42              |
| 1:AA:1082:A:H2'   | 1:AA:1083:U:C6    | 2.53                     | 0.42              |
| 3:AD:29:THR:O     | 3:AD:30:LYS:HB2   | 2.19                     | 0.42              |
| 7:AH:98:LEU:HD12  | 7:AH:98:LEU:N     | 2.34                     | 0.42              |
| 8:AI:49:GLN:HE21  | 8:AI:49:GLN:HB3   | 1.61                     | 0.42              |
| 12:AM:79:LEU:HD22 | 12:AM:86:ARG:NH2  | 2.33                     | 0.42              |
| 13:AN:15:LEU:C    | 13:AN:17:ASP:H    | 2.27                     | 0.42              |
| 15:AP:52:LEU:HG   | 15:AP:75:ILE:CG1  | 2.48                     | 0.42              |
| 16:AQ:28:VAL:O    | 16:AQ:28:VAL:HG13 | 2.19                     | 0.42              |
| 17:AR:46:THR:C    | 17:AR:48:ALA:H    | 2.28                     | 0.42              |
| 19:AT:60:GLN:HB2  | 19:AT:65:LEU:HD12 | 2.01                     | 0.42              |
| 19:AT:70:LYS:HA   | 19:AT:73:ARG:CZ   | 2.48                     | 0.42              |
| 23:BB:766:U:H2'   | 23:BB:767:U:H6    | 1.84                     | 0.42              |
| 23:BB:822:G:H2'   | 23:BB:823:C:H6    | 1.84                     | 0.42              |
| 23:BB:2082:A:H2'  | 23:BB:2083:G:O4'  | 2.19                     | 0.42              |
| 23:BB:2570:G:O2'  | 23:BB:2571:U:H5'  | 2.19                     | 0.42              |
| 23:BB:2637:U:O2'  | 23:BB:2638:G:H5'  | 2.18                     | 0.42              |
| 25:BC:27:LYS:HA   | 25:BC:79:ARG:NH2  | 2.34                     | 0.42              |
| 25:BC:84:PRO:O    | 25:BC:86:ARG:N    | 2.48                     | 0.42              |
| 27:BE:135:ALA:O   | 27:BE:139:LYS:HD2 | 2.19                     | 0.42              |
| 28:BF:177:ARG:HE  | 28:BF:178:LYS:HA  | 1.81                     | 0.42              |
| 30:BH:31:VAL:HB   | 30:BH:32:PRO:HD3  | 2.01                     | 0.42              |
| 30:BH:80:ILE:HD11 | 30:BH:102:ALA:HA  | 2.01                     | 0.42              |
| 31:BJ:81:ILE:CG1  | 31:BJ:82:GLY:N    | 2.69                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 33:BL:27:LEU:C     | 33:BL:29:LYS:N    | 2.70                     | 0.42              |
| 33:BL:77:ILE:C     | 33:BL:78:ARG:HG3  | 2.44                     | 0.42              |
| 33:BL:96:LYS:HD3   | 33:BL:96:LYS:N    | 2.34                     | 0.42              |
| 33:BL:127:VAL:HB   | 33:BL:128:THR:H   | 1.51                     | 0.42              |
| 34:BM:25:ASP:OD2   | 34:BM:66:ARG:NH2  | 2.52                     | 0.42              |
| 34:BM:36:VAL:HG11  | 34:BM:125:PRO:HD2 | 2.00                     | 0.42              |
| 36:BO:76:LYS:O     | 36:BO:77:ALA:C    | 2.62                     | 0.42              |
| 37:BP:25:VAL:HG12  | 37:BP:25:VAL:O    | 2.18                     | 0.42              |
| 37:BP:61:ARG:O     | 37:BP:63:ILE:N    | 2.52                     | 0.42              |
| 39:BR:39:LEU:O     | 39:BR:39:LEU:HD23 | 2.18                     | 0.42              |
| 39:BR:53:PHE:CD2   | 39:BR:55:ASP:N    | 2.82                     | 0.42              |
| 40:BS:9:HIS:C      | 40:BS:11:ARG:H    | 2.27                     | 0.42              |
| 41:BT:3:ARG:HG2    | 41:BT:7:LEU:HD23  | 2.01                     | 0.42              |
| 41:BT:32:LEU:C     | 41:BT:34:VAL:N    | 2.77                     | 0.42              |
| 41:BT:69:ARG:H     | 41:BT:75:GLY:CA   | 2.32                     | 0.42              |
| 42:BU:13:LEU:H     | 42:BU:68:ASN:HD21 | 1.66                     | 0.42              |
| 43:BW:9:THR:H      | 43:BW:10:ARG:HD3  | 1.83                     | 0.42              |
| 44:BX:19:LEU:C     | 44:BX:21:LEU:N    | 2.74                     | 0.42              |
| 46:BZ:58:ASP:OD2   | 46:BZ:63:ARG:NH1  | 2.52                     | 0.42              |
| 47:B0:53:VAL:HG12  | 47:B0:54:ILE:H    | 1.84                     | 0.42              |
| 52:BI:116:MET:CE   | 52:BI:127:SER:HB2 | 2.49                     | 0.42              |
| 1:CA:79:G:H2'      | 1:CA:80:A:C8      | 2.53                     | 0.42              |
| 1:CA:112:G:O2'     | 1:CA:113:G:H5'    | 2.19                     | 0.42              |
| 1:CA:1065:U:O2'    | 1:CA:1066:C:OP2   | 2.30                     | 0.42              |
| 1:CA:1493:A:C2'    | 1:CA:1494:G:OP2   | 2.67                     | 0.42              |
| 1:CA:1531:A:H2'    | 1:CA:1532:U:O4'   | 2.19                     | 0.42              |
| 2:CC:64:ARG:O      | 2:CC:65:VAL:HB    | 2.19                     | 0.42              |
| 2:CC:137:VAL:HG13  | 2:CC:148:ILE:CG2  | 2.49                     | 0.42              |
| 4:CE:89:THR:O      | 4:CE:91:SER:N     | 2.52                     | 0.42              |
| 5:CF:11:HIS:CD2    | 5:CF:13:ASP:HB3   | 2.54                     | 0.42              |
| 6:CG:46:LEU:O      | 6:CG:50:ALA:HB2   | 2.19                     | 0.42              |
| 9:CJ:84:VAL:O      | 9:CJ:88:MET:HB3   | 2.19                     | 0.42              |
| 10:CK:86:LYS:HG3   | 10:CK:113:THR:HA  | 2.00                     | 0.42              |
| 12:CM:68:LEU:HD23  | 12:CM:68:LEU:C    | 2.44                     | 0.42              |
| 15:CP:5:ARG:O      | 15:CP:19:VAL:HA   | 2.20                     | 0.42              |
| 15:CP:48:GLU:HG2   | 15:CP:49:GLY:N    | 2.34                     | 0.42              |
| 16:CQ:75:VAL:HG23  | 16:CQ:76:ARG:N    | 2.33                     | 0.42              |
| 20:CB:113:LEU:HD11 | 20:CB:144:GLU:HA  | 2.01                     | 0.42              |
| 20:CB:128:LEU:HD21 | 20:CB:132:GLU:HB3 | 2.01                     | 0.42              |
| 21:CU:19:LYS:HG3   | 21:CU:20:ARG:HE   | 1.83                     | 0.42              |
| 23:DB:96:C:H2'     | 23:DB:97:C:H6     | 1.84                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:329:G:H1'   | 23:DB:477:A:H1'    | 2.02                     | 0.42              |
| 23:DB:348:A:H2'   | 23:DB:349:U:O4'    | 2.18                     | 0.42              |
| 23:DB:543:G:C6    | 23:DB:544:C:H1'    | 2.54                     | 0.42              |
| 23:DB:679:C:O2'   | 23:DB:680:C:H5'    | 2.19                     | 0.42              |
| 23:DB:1068:G:C6   | 23:DB:1069:A:N6    | 2.87                     | 0.42              |
| 23:DB:1260:A:O2'  | 23:DB:1261:C:H5'   | 2.19                     | 0.42              |
| 23:DB:1818:U:C3'  | 25:DC:155:ARG:HB2  | 2.49                     | 0.42              |
| 23:DB:1869:G:HO2' | 23:DB:1871:A:H62   | 1.61                     | 0.42              |
| 23:DB:2087:G:H2'  | 23:DB:2088:A:H8    | 1.85                     | 0.42              |
| 23:DB:2508:G:O3'  | 23:DB:2555:U:H5'   | 2.18                     | 0.42              |
| 23:DB:2649:C:O2'  | 23:DB:2650:U:H5'   | 2.19                     | 0.42              |
| 23:DB:2866:U:O3'  | 23:DB:2867:G:H4'   | 2.19                     | 0.42              |
| 25:DC:62:ARG:HH22 | 25:DC:86:ARG:HH21  | 1.66                     | 0.42              |
| 25:DC:107:LYS:HD2 | 25:DC:196:ASN:HD21 | 1.84                     | 0.42              |
| 26:DD:154:LYS:O   | 26:DD:156:PHE:N    | 2.51                     | 0.42              |
| 27:DE:123:LYS:HD2 | 27:DE:157:LEU:CD1  | 2.48                     | 0.42              |
| 27:DE:146:VAL:O   | 27:DE:148:ILE:N    | 2.51                     | 0.42              |
| 27:DE:183:PHE:C   | 27:DE:185:LYS:N    | 2.75                     | 0.42              |
| 29:DG:23:ILE:HD13 | 29:DG:71:LEU:HD22  | 2.01                     | 0.42              |
| 29:DG:136:ASP:O   | 29:DG:140:ILE:HG12 | 2.19                     | 0.42              |
| 29:DG:154:GLU:OE2 | 29:DG:157:LYS:HB2  | 2.18                     | 0.42              |
| 31:DJ:80:HIS:O    | 31:DJ:81:ILE:C     | 2.62                     | 0.42              |
| 33:DL:77:ILE:CD1  | 33:DL:109:LYS:HB2  | 2.46                     | 0.42              |
| 34:DM:41:LEU:HD21 | 34:DM:46:ILE:HD11  | 2.01                     | 0.42              |
| 34:DM:43:ALA:HB3  | 34:DM:91:TYR:CD2   | 2.55                     | 0.42              |
| 35:DN:58:ASP:C    | 35:DN:60:VAL:H     | 2.27                     | 0.42              |
| 36:DO:31:THR:C    | 36:DO:33:ARG:N     | 2.76                     | 0.42              |
| 37:DP:18:SER:C    | 37:DP:20:ARG:H     | 2.27                     | 0.42              |
| 37:DP:92:ARG:HD3  | 37:DP:110:LYS:O    | 2.19                     | 0.42              |
| 38:DQ:3:VAL:O     | 38:DQ:4:LYS:C      | 2.61                     | 0.42              |
| 38:DQ:90:ASP:CB   | 39:DR:42:ALA:HB3   | 2.49                     | 0.42              |
| 42:DU:71:ILE:HD13 | 42:DU:71:ILE:C     | 2.44                     | 0.42              |
| 44:DX:46:VAL:O    | 44:DX:49:ASP:HB3   | 2.18                     | 0.42              |
| 47:D0:15:ARG:CZ   | 47:D0:15:ARG:HB3   | 2.49                     | 0.42              |
| 51:D4:24:ARG:NE   | 51:D4:37:GLN:HA    | 2.33                     | 0.42              |
| 1:AA:234:C:H2'    | 1:AA:235:C:H6      | 1.84                     | 0.42              |
| 1:AA:254:G:OP1    | 16:AQ:68:LYS:O     | 2.37                     | 0.42              |
| 1:AA:664:G:H5''   | 17:AR:52:ARG:NH2   | 2.34                     | 0.42              |
| 1:AA:844:G:H2'    | 1:AA:845:A:H5''    | 2.01                     | 0.42              |
| 1:AA:1250:A:H5'   | 8:AI:69:GLY:O      | 2.18                     | 0.42              |
| 1:AA:1273:C:H2'   | 1:AA:1274:A:O4'    | 2.19                     | 0.42              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:AC:110:LEU:HB3  | 2:AC:203:LYS:NZ    | 2.32                     | 0.42              |
| 3:AD:116:LEU:O    | 3:AD:121:ALA:HB3   | 2.19                     | 0.42              |
| 5:AF:43:GLY:HA2   | 5:AF:58:HIS:CE1    | 2.53                     | 0.42              |
| 6:AG:102:TRP:CD1  | 6:AG:102:TRP:N     | 2.86                     | 0.42              |
| 7:AH:38:VAL:O     | 7:AH:42:GLU:HG2    | 2.19                     | 0.42              |
| 8:AI:118:ARG:NH1  | 8:AI:122:ARG:HE    | 2.17                     | 0.42              |
| 9:AJ:38:GLY:O     | 9:AJ:74:VAL:HA     | 2.19                     | 0.42              |
| 13:AN:62:ARG:HA   | 13:AN:69:PRO:HA    | 2.01                     | 0.42              |
| 20:AB:112:ARG:HG3 | 20:AB:112:ARG:HH11 | 1.83                     | 0.42              |
| 23:BB:647:G:H2'   | 23:BB:648:G:C8     | 2.55                     | 0.42              |
| 23:BB:795:C:H2'   | 23:BB:796:C:H6     | 1.85                     | 0.42              |
| 23:BB:935:C:H2'   | 23:BB:936:A:C8     | 2.54                     | 0.42              |
| 23:BB:1017:G:O2'  | 23:BB:1018:U:H5'   | 2.20                     | 0.42              |
| 23:BB:1064:C:H2'  | 23:BB:1065:U:O4'   | 2.19                     | 0.42              |
| 23:BB:1236:G:O2'  | 23:BB:1237:A:P     | 2.77                     | 0.42              |
| 23:BB:1270:C:H5'' | 23:BB:1271:G:O5'   | 2.19                     | 0.42              |
| 23:BB:1370:C:H2'  | 23:BB:1371:G:O4'   | 2.18                     | 0.42              |
| 23:BB:1408:G:H2'  | 23:BB:1409:U:C6    | 2.54                     | 0.42              |
| 23:BB:1421:G:C2   | 23:BB:1422:G:C8    | 3.07                     | 0.42              |
| 23:BB:1803:A:H2   | 23:BB:1823:G:O4'   | 2.02                     | 0.42              |
| 23:BB:2361:G:O2'  | 23:BB:2362:C:H5'   | 2.19                     | 0.42              |
| 23:BB:2643:G:H2'  | 23:BB:2644:G:O4'   | 2.18                     | 0.42              |
| 23:BB:2649:C:H2'  | 23:BB:2650:U:C6    | 2.52                     | 0.42              |
| 24:BV:53:LYS:HE3  | 24:BV:55:GLU:OE2   | 2.19                     | 0.42              |
| 25:BC:68:ARG:CZ   | 25:BC:103:ILE:HD12 | 2.49                     | 0.42              |
| 25:BC:124:LYS:O   | 25:BC:191:LEU:CD1  | 2.67                     | 0.42              |
| 25:BC:171:VAL:HB  | 25:BC:182:LYS:CB   | 2.47                     | 0.42              |
| 26:BD:31:ALA:HA   | 26:BD:51:THR:HG1   | 1.82                     | 0.42              |
| 26:BD:37:VAL:HG22 | 26:BD:46:ARG:HD3   | 2.00                     | 0.42              |
| 27:BE:4:VAL:N     | 27:BE:117:ARG:HH21 | 2.17                     | 0.42              |
| 27:BE:120:VAL:H   | 27:BE:189:THR:HA   | 1.84                     | 0.42              |
| 27:BE:141:MET:C   | 27:BE:143:LEU:H    | 2.26                     | 0.42              |
| 27:BE:148:ILE:N   | 27:BE:183:PHE:HD2  | 2.17                     | 0.42              |
| 28:BF:133:GLU:CG  | 28:BF:147:ARG:HG2  | 2.32                     | 0.42              |
| 29:BG:150:TYR:O   | 29:BG:151:ARG:HB2  | 2.19                     | 0.42              |
| 30:BH:4:ILE:N     | 30:BH:37:VAL:HB    | 2.19                     | 0.42              |
| 30:BH:5:LEU:O     | 30:BH:6:LEU:HB3    | 2.19                     | 0.42              |
| 31:BJ:55:ILE:HD13 | 31:BJ:132:HIS:NE2  | 2.35                     | 0.42              |
| 31:BJ:72:LYS:HG3  | 31:BJ:90:GLU:HB2   | 2.01                     | 0.42              |
| 31:BJ:100:VAL:CG2 | 31:BJ:101:ILE:H    | 2.26                     | 0.42              |
| 32:BK:104:THR:OG1 | 32:BK:107:LEU:HB2  | 2.19                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:BM:33:LEU:HB2  | 34:BM:101:VAL:CG1 | 2.50                     | 0.42              |
| 34:BM:90:GLU:O    | 34:BM:91:TYR:HB2  | 2.20                     | 0.42              |
| 35:BN:28:LEU:CD2  | 35:BN:48:VAL:HG21 | 2.49                     | 0.42              |
| 35:BN:51:LEU:HA   | 35:BN:54:LEU:HD13 | 2.00                     | 0.42              |
| 37:BP:91:VAL:HB   | 37:BP:113:LEU:CG  | 2.47                     | 0.42              |
| 39:BR:33:VAL:HG12 | 39:BR:33:VAL:O    | 2.19                     | 0.42              |
| 40:BS:56:ALA:C    | 40:BS:58:ALA:N    | 2.76                     | 0.42              |
| 42:BU:38:ILE:O    | 42:BU:62:ALA:HB3  | 2.19                     | 0.42              |
| 43:BW:11:ASN:ND2  | 43:BW:13:ARG:NH2  | 2.67                     | 0.42              |
| 44:BX:41:HIS:CD2  | 44:BX:41:HIS:H    | 2.36                     | 0.42              |
| 44:BX:55:THR:HG22 | 44:BX:59:GLU:CD   | 2.44                     | 0.42              |
| 47:B0:11:LYS:HG3  | 47:B0:12:ARG:N    | 2.35                     | 0.42              |
| 50:B3:9:ALA:O     | 50:B3:13:PHE:HB3  | 2.19                     | 0.42              |
| 52:BI:80:LYS:HG3  | 52:BI:135:MET:HE1 | 2.01                     | 0.42              |
| 1:CA:138:G:O2'    | 1:CA:139:A:H5'    | 2.19                     | 0.42              |
| 1:CA:195:A:H1'    | 1:CA:222:C:O2'    | 2.18                     | 0.42              |
| 1:CA:233:C:O2'    | 1:CA:234:C:H5'    | 2.19                     | 0.42              |
| 1:CA:329:A:H5'    | 1:CA:329:A:H8     | 1.84                     | 0.42              |
| 1:CA:599:C:H4'    | 7:CH:121:GLY:C    | 2.44                     | 0.42              |
| 1:CA:626:G:H2'    | 1:CA:627:G:H8     | 1.83                     | 0.42              |
| 1:CA:674:G:OP1    | 5:CF:51:ILE:HG13  | 2.20                     | 0.42              |
| 1:CA:806:C:O2'    | 1:CA:807:A:H5'    | 2.20                     | 0.42              |
| 1:CA:913:A:H4'    | 1:CA:914:A:H4'    | 2.01                     | 0.42              |
| 2:CC:128:MET:O    | 2:CC:130:ARG:N    | 2.41                     | 0.42              |
| 2:CC:139:ASN:O    | 2:CC:143:LEU:HD13 | 2.18                     | 0.42              |
| 3:CD:24:VAL:HG23  | 3:CD:25:ARG:H     | 1.83                     | 0.42              |
| 4:CE:102:THR:HG21 | 4:CE:123:LEU:HD21 | 2.01                     | 0.42              |
| 7:CH:14:ARG:HG3   | 7:CH:15:ASN:N     | 2.33                     | 0.42              |
| 9:CJ:52:LEU:CD1   | 9:CJ:62:ARG:HE    | 2.31                     | 0.42              |
| 13:CN:63:CYS:O    | 13:CN:67:GLY:HA2  | 2.18                     | 0.42              |
| 15:CP:18:GLN:HA   | 15:CP:38:PHE:HA   | 2.02                     | 0.42              |
| 19:CT:66:ILE:HG22 | 19:CT:67:HIS:N    | 2.34                     | 0.42              |
| 22:DA:15:A:H1'    | 22:DA:109:A:C5    | 2.55                     | 0.42              |
| 22:DA:43:C:C4'    | 28:DF:62:GLN:HE21 | 2.32                     | 0.42              |
| 22:DA:56:G:H4'    | 22:DA:57:A:H5'    | 2.02                     | 0.42              |
| 23:DB:5:A:H2'     | 23:DB:6:A:H8      | 1.84                     | 0.42              |
| 23:DB:125:A:C4'   | 49:D2:13:ASN:ND2  | 2.82                     | 0.42              |
| 23:DB:249:C:O3'   | 50:D3:7:ARG:HD3   | 2.19                     | 0.42              |
| 23:DB:538:A:H2'   | 23:DB:539:G:O4'   | 2.19                     | 0.42              |
| 23:DB:545:U:C4    | 23:DB:548:G:OP1   | 2.73                     | 0.42              |
| 23:DB:678:C:H2'   | 23:DB:679:C:C6    | 2.53                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DB:906:U:H1'   | 34:DM:66:ARG:NH2  | 2.34                     | 0.42              |
| 23:DB:1027:A:C2   | 23:DB:2488:G:H5'' | 2.53                     | 0.42              |
| 23:DB:1213:A:H62  | 23:DB:1236:G:H1'  | 1.83                     | 0.42              |
| 23:DB:1526:C:O2'  | 23:DB:1527:G:H5'  | 2.19                     | 0.42              |
| 23:DB:1813:G:O4'  | 25:DC:45:ASN:HB3  | 2.20                     | 0.42              |
| 23:DB:2019:A:C6   | 23:DB:2020:A:N7   | 2.88                     | 0.42              |
| 23:DB:2479:U:O5'  | 23:DB:2479:U:H6   | 2.02                     | 0.42              |
| 23:DB:2561:U:O3'  | 32:DK:40:LYS:HE2  | 2.19                     | 0.42              |
| 23:DB:2633:G:H2'  | 23:DB:2634:A:O4'  | 2.19                     | 0.42              |
| 23:DB:2671:G:O2'  | 23:DB:2672:U:H5'  | 2.19                     | 0.42              |
| 23:DB:2686:G:H2'  | 23:DB:2687:U:O4'  | 2.19                     | 0.42              |
| 23:DB:2705:A:H2'  | 23:DB:2706:A:O4'  | 2.19                     | 0.42              |
| 25:DC:47:ARG:HB3  | 25:DC:48:ILE:H    | 1.54                     | 0.42              |
| 27:DE:115:GLN:CB  | 27:DE:117:ARG:NH1 | 2.81                     | 0.42              |
| 29:DG:171:LYS:C   | 29:DG:171:LYS:CD  | 2.92                     | 0.42              |
| 30:DH:88:GLY:HA3  | 30:DH:125:THR:OG1 | 2.18                     | 0.42              |
| 30:DH:108:VAL:CG1 | 30:DH:110:VAL:HB  | 2.49                     | 0.42              |
| 31:DJ:78:THR:H    | 31:DJ:84:ILE:HD13 | 1.84                     | 0.42              |
| 33:DL:37:GLY:C    | 33:DL:38:GLN:HG3  | 2.44                     | 0.42              |
| 33:DL:71:ALA:O    | 33:DL:72:ALA:O    | 2.37                     | 0.42              |
| 37:DP:18:SER:HB2  | 37:DP:87:ARG:NH1  | 2.34                     | 0.42              |
| 41:DT:69:ARG:HG2  | 41:DT:69:ARG:NH1  | 2.34                     | 0.42              |
| 42:DU:32:LYS:HA   | 42:DU:65:GLN:NE2  | 2.34                     | 0.42              |
| 44:DX:55:THR:C    | 44:DX:57:LEU:N    | 2.77                     | 0.42              |
| 48:D1:5:ARG:HA    | 48:D1:28:THR:HG1  | 1.83                     | 0.42              |
| 48:D1:8:ILE:HG21  | 48:D1:27:ARG:HD3  | 2.01                     | 0.42              |
| 1:AA:154:U:O2'    | 1:AA:155:A:H5'    | 2.20                     | 0.42              |
| 1:AA:492:C:C3'    | 1:AA:493:A:H5''   | 2.49                     | 0.42              |
| 1:AA:1073:U:H2'   | 1:AA:1074:G:H8    | 1.84                     | 0.42              |
| 1:AA:1073:U:C2    | 1:AA:1074:G:C8    | 3.08                     | 0.42              |
| 1:AA:1178:G:N2    | 1:AA:1181:G:C8    | 2.87                     | 0.42              |
| 3:AD:117:VAL:C    | 3:AD:130:ASN:HA   | 2.43                     | 0.42              |
| 4:AE:109:ALA:CB   | 4:AE:135:VAL:HG23 | 2.47                     | 0.42              |
| 5:AF:29:ILE:HG21  | 5:AF:64:VAL:CG1   | 2.50                     | 0.42              |
| 6:AG:37:THR:O     | 6:AG:41:ILE:HB    | 2.19                     | 0.42              |
| 6:AG:90:VAL:HG23  | 6:AG:90:VAL:O     | 2.19                     | 0.42              |
| 10:AK:62:ALA:O    | 10:AK:65:ALA:HB3  | 2.19                     | 0.42              |
| 14:AO:38:LEU:HB3  | 14:AO:42:PHE:CE1  | 2.55                     | 0.42              |
| 23:BB:312:G:C2    | 23:BB:313:G:C8    | 3.07                     | 0.42              |
| 23:BB:500:G:OP1   | 42:BU:40:LEU:HG   | 2.19                     | 0.42              |
| 23:BB:651:G:OP1   | 50:B3:16:THR:HB   | 2.20                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:748:G:OP2    | 40:BS:88:ARG:HD3   | 2.19                     | 0.42              |
| 23:BB:970:U:H2'    | 23:BB:971:G:C8     | 2.55                     | 0.42              |
| 23:BB:1114:C:H2'   | 23:BB:1115:G:C8    | 2.55                     | 0.42              |
| 23:BB:1221:C:O2'   | 23:BB:1222:U:H5'   | 2.19                     | 0.42              |
| 23:BB:1225:G:C5'   | 39:BR:78:ARG:HH22  | 2.27                     | 0.42              |
| 23:BB:1401:G:H2'   | 23:BB:1402:U:C6    | 2.54                     | 0.42              |
| 23:BB:1498:C:H2'   | 23:BB:1499:C:C6    | 2.54                     | 0.42              |
| 23:BB:1513:U:O2'   | 23:BB:1514:G:H5'   | 2.19                     | 0.42              |
| 23:BB:1674:G:N2    | 23:BB:1677:A:N1    | 2.68                     | 0.42              |
| 23:BB:1685:C:H2'   | 23:BB:1686:C:C6    | 2.54                     | 0.42              |
| 23:BB:1791:A:H1'   | 25:BC:206:LYS:HZ1  | 1.81                     | 0.42              |
| 23:BB:1804:C:P     | 25:BC:254:LYS:HG2  | 2.58                     | 0.42              |
| 23:BB:1891:G:H2'   | 23:BB:1892:C:H6    | 1.84                     | 0.42              |
| 23:BB:2285:C:N4    | 48:B1:24:LYS:HZ2   | 2.18                     | 0.42              |
| 23:BB:2559:C:O2'   | 23:BB:2560:A:H5'   | 2.19                     | 0.42              |
| 23:BB:2705:A:H2'   | 23:BB:2706:A:O4'   | 2.19                     | 0.42              |
| 23:BB:2811:G:H2'   | 23:BB:2812:G:C8    | 2.54                     | 0.42              |
| 23:BB:2813:A:O2'   | 23:BB:2814:A:H5'   | 2.18                     | 0.42              |
| 25:BC:170:TYR:HA   | 25:BC:185:ALA:HB2  | 2.01                     | 0.42              |
| 26:BD:205:PRO:O    | 26:BD:206:ALA:HB2  | 2.19                     | 0.42              |
| 27:BE:53:THR:O     | 27:BE:55:SER:N     | 2.52                     | 0.42              |
| 30:BH:124:THR:HG22 | 30:BH:125:THR:N    | 2.35                     | 0.42              |
| 31:BJ:68:LYS:CA    | 31:BJ:71:ASP:OD1   | 2.65                     | 0.42              |
| 33:BL:58:TYR:CD2   | 33:BL:58:TYR:N     | 2.84                     | 0.42              |
| 34:BM:3:GLN:CG     | 34:BM:46:ILE:HB    | 2.43                     | 0.42              |
| 34:BM:86:LYS:HB3   | 34:BM:87:GLY:H     | 1.67                     | 0.42              |
| 35:BN:28:LEU:CD2   | 35:BN:113:ILE:HG21 | 2.49                     | 0.42              |
| 37:BP:47:ILE:HG22  | 37:BP:48:ALA:N     | 2.17                     | 0.42              |
| 37:BP:77:SER:N     | 37:BP:78:PRO:CD    | 2.73                     | 0.42              |
| 39:BR:101:ILE:HB   | 39:BR:102:SER:H    | 1.69                     | 0.42              |
| 41:BT:64:LYS:HZ2   | 41:BT:79:ASP:HB2   | 1.85                     | 0.42              |
| 42:BU:21:ARG:HG2   | 42:BU:21:ARG:NH1   | 2.33                     | 0.42              |
| 43:BW:44:PHE:HB3   | 43:BW:76:ARG:CB    | 2.49                     | 0.42              |
| 44:BX:29:ARG:O     | 44:BX:30:MET:C     | 2.63                     | 0.42              |
| 46:BZ:9:TYR:C      | 46:BZ:11:GLU:N     | 2.76                     | 0.42              |
| 47:B0:2:VAL:CG2    | 47:B0:3:GLN:H      | 2.33                     | 0.42              |
| 50:B3:16:THR:CG2   | 50:B3:22:LYS:HG2   | 2.50                     | 0.42              |
| 52:BI:63:ASP:O     | 52:BI:65:SER:N     | 2.53                     | 0.42              |
| 1:CA:349:A:H2'     | 1:CA:350:G:C8      | 2.54                     | 0.42              |
| 1:CA:538:G:H2'     | 1:CA:539:A:H8      | 1.85                     | 0.42              |
| 1:CA:838:G:H2'     | 1:CA:839:C:O4'     | 2.20                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:976:G:OP2     | 1:CA:1358:U:O2'    | 2.32                     | 0.42              |
| 1:CA:1141:C:H2'    | 1:CA:1142:G:H8     | 1.83                     | 0.42              |
| 1:CA:1306:A:C2'    | 1:CA:1307:U:H5'    | 2.49                     | 0.42              |
| 1:CA:1394:A:OP1    | 1:CA:1394:A:H8     | 2.03                     | 0.42              |
| 2:CC:130:ARG:HA    | 2:CC:130:ARG:HD2   | 1.86                     | 0.42              |
| 2:CC:172:VAL:O     | 2:CC:174:LEU:HD12  | 2.19                     | 0.42              |
| 2:CC:182:ASP:CB    | 2:CC:203:LYS:HE2   | 2.43                     | 0.42              |
| 2:CC:183:TYR:HA    | 2:CC:199:VAL:O     | 2.19                     | 0.42              |
| 3:CD:159:GLU:O     | 3:CD:162:GLU:HG2   | 2.19                     | 0.42              |
| 4:CE:105:ILE:HD12  | 4:CE:123:LEU:CD2   | 2.50                     | 0.42              |
| 6:CG:147:ASN:C     | 6:CG:149:ALA:N     | 2.76                     | 0.42              |
| 8:CI:49:GLN:O      | 8:CI:53:LEU:HD23   | 2.19                     | 0.42              |
| 17:CR:28:LEU:C     | 17:CR:30:ASN:H     | 2.27                     | 0.42              |
| 18:CS:66:VAL:C     | 18:CS:68:HIS:H     | 2.27                     | 0.42              |
| 19:CT:79:THR:O     | 19:CT:82:ILE:HG12  | 2.19                     | 0.42              |
| 20:CB:15:PHE:HB2   | 20:CB:16:GLY:H     | 1.65                     | 0.42              |
| 20:CB:61:SER:OG    | 20:CB:62:ARG:HD2   | 2.19                     | 0.42              |
| 23:DB:533:G:N3     | 38:DQ:40:LYS:CG    | 2.82                     | 0.42              |
| 23:DB:539:G:H2'    | 23:DB:540:C:H6     | 1.83                     | 0.42              |
| 23:DB:662:G:H5'    | 33:DL:26:GLY:H     | 1.83                     | 0.42              |
| 23:DB:756:A:H2'    | 23:DB:757:G:O4'    | 2.20                     | 0.42              |
| 23:DB:954:G:O2'    | 23:DB:2274:A:N1    | 2.44                     | 0.42              |
| 23:DB:1220:G:H2'   | 23:DB:1221:C:H6    | 1.83                     | 0.42              |
| 23:DB:1252:G:H21   | 38:DQ:32:ARG:CZ    | 2.32                     | 0.42              |
| 23:DB:1401:G:H2'   | 23:DB:1402:U:C6    | 2.54                     | 0.42              |
| 23:DB:2010:G:H5''  | 40:DS:42:LYS:HB3   | 2.00                     | 0.42              |
| 23:DB:2082:A:N6    | 23:DB:2237:G:H1'   | 2.34                     | 0.42              |
| 23:DB:2248:C:H3'   | 23:DB:2249:U:C6    | 2.55                     | 0.42              |
| 23:DB:2259:U:C6    | 23:DB:2427:C:C4    | 3.07                     | 0.42              |
| 23:DB:2393:U:C5    | 50:D3:30:HIS:HE1   | 2.37                     | 0.42              |
| 23:DB:2408:U:H2'   | 23:DB:2409:G:C8    | 2.54                     | 0.42              |
| 23:DB:2462:C:H2'   | 23:DB:2463:C:H6    | 1.84                     | 0.42              |
| 23:DB:2570:G:O2'   | 23:DB:2571:U:H5'   | 2.20                     | 0.42              |
| 23:DB:2821:A:OP2   | 26:DD:115:GLY:O    | 2.38                     | 0.42              |
| 24:DV:9:ARG:CZ     | 24:DV:20:LEU:HD11  | 2.50                     | 0.42              |
| 25:DC:163:ILE:HG12 | 25:DC:173:LEU:HD23 | 2.01                     | 0.42              |
| 25:DC:247:TRP:HZ2  | 25:DC:254:LYS:HZ3  | 1.67                     | 0.42              |
| 26:DD:48:ILE:HG22  | 26:DD:49:GLN:H     | 1.80                     | 0.42              |
| 27:DE:112:LEU:O    | 27:DE:113:VAL:HB   | 2.20                     | 0.42              |
| 30:DH:4:ILE:HD11   | 30:DH:37:VAL:CA    | 2.48                     | 0.42              |
| 30:DH:35:LYS:HB2   | 30:DH:35:LYS:HE2   | 1.91                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 30:DH:132:PHE:HE2 | 30:DH:134:VAL:HG22 | 1.84                     | 0.42              |
| 31:DJ:7:LYS:N     | 31:DJ:8:PRO:CD     | 2.82                     | 0.42              |
| 31:DJ:15:TRP:CB   | 31:DJ:139:VAL:HA   | 2.49                     | 0.42              |
| 31:DJ:81:ILE:C    | 31:DJ:83:GLY:N     | 2.77                     | 0.42              |
| 31:DJ:110:PRO:O   | 31:DJ:111:LYS:HB2  | 2.18                     | 0.42              |
| 32:DK:43:ILE:HG12 | 32:DK:52:VAL:CG1   | 2.46                     | 0.42              |
| 33:DL:63:LYS:CB   | 50:D3:26:ALA:HB2   | 2.47                     | 0.42              |
| 33:DL:77:ILE:O    | 33:DL:110:VAL:O    | 2.37                     | 0.42              |
| 33:DL:81:ASP:O    | 33:DL:85:VAL:HG12  | 2.19                     | 0.42              |
| 34:DM:41:LEU:CD2  | 34:DM:46:ILE:HD11  | 2.49                     | 0.42              |
| 36:DO:31:THR:C    | 36:DO:33:ARG:H     | 2.27                     | 0.42              |
| 36:DO:82:ALA:HB1  | 36:DO:87:ILE:HG21  | 2.01                     | 0.42              |
| 38:DQ:44:TYR:O    | 38:DQ:48:ASP:N     | 2.51                     | 0.42              |
| 43:DW:67:LYS:CD   | 43:DW:69:GLU:H     | 2.33                     | 0.42              |
| 45:DY:43:ILE:O    | 45:DY:47:ILE:HG13  | 2.20                     | 0.42              |
| 47:D0:27:LEU:O    | 47:D0:38:LEU:HD13  | 2.19                     | 0.42              |
| 50:D3:57:VAL:HG22 | 50:D3:57:VAL:O     | 2.19                     | 0.42              |
| 1:AA:15:G:O2'     | 4:AE:28:ARG:HD2    | 2.20                     | 0.42              |
| 1:AA:123:U:H2'    | 1:AA:124:C:C6      | 2.54                     | 0.42              |
| 1:AA:128:G:O2'    | 1:AA:129:A:H5'     | 2.18                     | 0.42              |
| 1:AA:138:G:O2'    | 1:AA:139:A:H5'     | 2.19                     | 0.42              |
| 1:AA:329:A:H8     | 1:AA:329:A:H5'     | 1.84                     | 0.42              |
| 1:AA:343:U:O2'    | 1:AA:344:A:H2'     | 2.20                     | 0.42              |
| 1:AA:442:G:H2'    | 1:AA:443:C:H6      | 1.84                     | 0.42              |
| 1:AA:913:A:H4'    | 1:AA:914:A:O5'     | 2.19                     | 0.42              |
| 1:AA:1065:U:C1'   | 1:AA:1066:C:OP2    | 2.66                     | 0.42              |
| 1:AA:1306:A:C2    | 1:AA:1332:A:N9     | 2.87                     | 0.42              |
| 3:AD:173:ASP:HB3  | 3:AD:178:GLU:HB3   | 2.01                     | 0.42              |
| 3:AD:191:SER:O    | 3:AD:192:ALA:CB    | 2.68                     | 0.42              |
| 6:AG:45:ALA:HB1   | 6:AG:120:ALA:HB2   | 2.00                     | 0.42              |
| 7:AH:92:PRO:HA    | 7:AH:93:LYS:NZ     | 2.32                     | 0.42              |
| 8:AI:119:LYS:C    | 8:AI:121:ARG:H     | 2.27                     | 0.42              |
| 13:AN:12:ARG:HH11 | 13:AN:60:ARG:HH12  | 1.64                     | 0.42              |
| 18:AS:35:ARG:HG2  | 18:AS:50:VAL:CG1   | 2.49                     | 0.42              |
| 23:BB:84:A:N6     | 23:BB:99:U:H5'     | 2.35                     | 0.42              |
| 23:BB:126:A:O5'   | 49:B2:19:ARG:HB3   | 2.19                     | 0.42              |
| 23:BB:299:A:N6    | 23:BB:322:A:O2'    | 2.49                     | 0.42              |
| 23:BB:453:A:H4'   | 23:BB:472:A:H62    | 1.84                     | 0.42              |
| 23:BB:679:C:O2'   | 23:BB:680:C:H5'    | 2.19                     | 0.42              |
| 23:BB:693:A:H2'   | 23:BB:694:U:C6     | 2.54                     | 0.42              |
| 23:BB:919:U:O5'   | 23:BB:919:U:H6     | 2.03                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BB:1173:U:H2'  | 23:BB:1174:U:H4'  | 2.00                     | 0.42              |
| 23:BB:1298:C:O2'  | 23:BB:1301:A:O2'  | 2.36                     | 0.42              |
| 23:BB:1566:A:C6   | 25:BC:213:ARG:CZ  | 3.02                     | 0.42              |
| 23:BB:1604:C:H5'' | 55:BB:3376:HOH:O  | 2.18                     | 0.42              |
| 23:BB:1770:G:O2'  | 23:BB:1771:C:H5'  | 2.19                     | 0.42              |
| 23:BB:2263:C:H4'  | 23:BB:2329:U:H4'  | 2.01                     | 0.42              |
| 23:BB:2333:A:HO2' | 36:BO:7:ARG:HD3   | 1.84                     | 0.42              |
| 23:BB:2463:C:O2'  | 23:BB:2464:G:H5'  | 2.19                     | 0.42              |
| 23:BB:2484:G:HO2' | 34:BM:45:GLN:NE2  | 2.18                     | 0.42              |
| 25:BC:27:LYS:O    | 25:BC:28:PRO:C    | 2.63                     | 0.42              |
| 27:BE:68:ALA:O    | 27:BE:69:ARG:HB3  | 2.20                     | 0.42              |
| 27:BE:108:ILE:O   | 27:BE:109:LEU:C   | 2.62                     | 0.42              |
| 27:BE:112:LEU:O   | 27:BE:116:ASP:N   | 2.52                     | 0.42              |
| 30:BH:90:LEU:HD13 | 30:BH:123:ARG:O   | 2.19                     | 0.42              |
| 31:BJ:12:LYS:O    | 31:BJ:13:ARG:HG3  | 2.19                     | 0.42              |
| 31:BJ:45:THR:CB   | 38:BQ:63:ARG:HH22 | 2.16                     | 0.42              |
| 31:BJ:124:VAL:O   | 31:BJ:125:TYR:HB2 | 2.18                     | 0.42              |
| 32:BK:2:ILE:N     | 32:BK:33:ALA:N    | 2.68                     | 0.42              |
| 32:BK:71:ARG:HH11 | 32:BK:71:ARG:HG2  | 1.84                     | 0.42              |
| 33:BL:13:LYS:C    | 33:BL:15:ALA:H    | 2.27                     | 0.42              |
| 33:BL:17:LYS:HA   | 33:BL:17:LYS:HD3  | 1.92                     | 0.42              |
| 33:BL:56:PRO:O    | 33:BL:57:LEU:C    | 2.62                     | 0.42              |
| 33:BL:78:ARG:NH1  | 33:BL:78:ARG:O    | 2.53                     | 0.42              |
| 34:BM:3:GLN:HE21  | 34:BM:3:GLN:HB2   | 1.67                     | 0.42              |
| 37:BP:61:ARG:CB   | 37:BP:61:ARG:NH1  | 2.81                     | 0.42              |
| 38:BQ:63:ARG:HG3  | 38:BQ:64:ILE:N    | 2.33                     | 0.42              |
| 38:BQ:89:ILE:O    | 38:BQ:89:ILE:HG23 | 2.20                     | 0.42              |
| 39:BR:41:ILE:HD13 | 39:BR:43:ASN:HA   | 2.00                     | 0.42              |
| 39:BR:51:VAL:HG13 | 39:BR:52:PRO:HD2  | 2.01                     | 0.42              |
| 42:BU:70:ALA:O    | 42:BU:72:PHE:N    | 2.53                     | 0.42              |
| 45:BY:22:THR:O    | 45:BY:26:LEU:N    | 2.53                     | 0.42              |
| 46:BZ:2:LYS:HB2   | 46:BZ:3:LYS:H     | 1.69                     | 0.42              |
| 47:B0:26:SER:HB2  | 47:B0:38:LEU:CD1  | 2.46                     | 0.42              |
| 48:B1:29:LYS:O    | 48:B1:30:PRO:C    | 2.62                     | 0.42              |
| 48:B1:51:ALA:HB3  | 48:B1:52:LYS:HD2  | 2.01                     | 0.42              |
| 51:B4:12:ARG:H    | 51:B4:12:ARG:CD   | 2.06                     | 0.42              |
| 52:BI:21:PRO:HB2  | 52:BI:22:PRO:CD   | 2.44                     | 0.42              |
| 1:CA:6:G:H4'      | 1:CA:298:A:H4'    | 2.01                     | 0.42              |
| 1:CA:64:G:H4'     | 1:CA:65:A:H5''    | 2.01                     | 0.42              |
| 1:CA:113:G:O4'    | 1:CA:354:G:H4'    | 2.19                     | 0.42              |
| 1:CA:167:A:O2'    | 1:CA:168:G:H5'    | 2.19                     | 0.42              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:492:C:C3'     | 1:CA:493:A:H5''    | 2.50                     | 0.42              |
| 1:CA:1164:G:H2'    | 1:CA:1165:U:H6     | 1.85                     | 0.42              |
| 1:CA:1237:C:O4'    | 1:CA:1334:G:N2     | 2.50                     | 0.42              |
| 1:CA:1250:A:H5''   | 8:CI:68:GLY:HA2    | 2.01                     | 0.42              |
| 1:CA:1252:A:H4'    | 1:CA:1369:C:H4'    | 2.01                     | 0.42              |
| 2:CC:45:GLU:C      | 2:CC:46:LEU:HD23   | 2.44                     | 0.42              |
| 4:CE:10:LEU:O      | 4:CE:10:LEU:HD12   | 2.20                     | 0.42              |
| 5:CF:15:SER:HA     | 5:CF:18:VAL:HG23   | 2.01                     | 0.42              |
| 5:CF:84:VAL:HG22   | 5:CF:85:ILE:H      | 1.85                     | 0.42              |
| 8:CI:19:PHE:O      | 8:CI:62:LEU:HA     | 2.19                     | 0.42              |
| 8:CI:44:ARG:C      | 8:CI:46:VAL:H      | 2.28                     | 0.42              |
| 8:CI:94:ARG:HG3    | 8:CI:98:ARG:NH2    | 2.33                     | 0.42              |
| 9:CJ:66:GLU:HG2    | 9:CJ:67:ILE:N      | 2.34                     | 0.42              |
| 11:CL:66:ILE:HG21  | 11:CL:71:HIS:HB3   | 2.00                     | 0.42              |
| 18:CS:20:LYS:HD2   | 18:CS:20:LYS:C     | 2.44                     | 0.42              |
| 20:CB:86:CYS:HB3   | 20:CB:88:GLN:CG    | 2.49                     | 0.42              |
| 21:CU:36:PHE:HB2   | 21:CU:39:LYS:CB    | 2.47                     | 0.42              |
| 23:DB:62:U:H3'     | 23:DB:63:A:C8      | 2.54                     | 0.42              |
| 23:DB:222:A:N1     | 23:DB:233:A:H5''   | 2.35                     | 0.42              |
| 23:DB:372:G:N7     | 46:DZ:57:VAL:HG21  | 2.34                     | 0.42              |
| 23:DB:1189:A:H2'   | 23:DB:1190:G:H5'   | 2.02                     | 0.42              |
| 23:DB:1290:C:O2'   | 23:DB:1291:C:H5'   | 2.19                     | 0.42              |
| 23:DB:1294:U:C4    | 23:DB:1295:C:C5    | 3.07                     | 0.42              |
| 23:DB:1314:C:H2'   | 23:DB:1314:C:O2    | 2.18                     | 0.42              |
| 23:DB:1592:C:H2'   | 23:DB:1593:A:H8    | 1.84                     | 0.42              |
| 23:DB:1829:A:H3'   | 23:DB:1830:C:C6    | 2.55                     | 0.42              |
| 23:DB:2153:C:H2'   | 23:DB:2154:A:H8    | 1.84                     | 0.42              |
| 23:DB:2259:U:O2'   | 23:DB:2260:C:H5'   | 2.19                     | 0.42              |
| 23:DB:2282:G:O2'   | 23:DB:2283:C:OP2   | 2.37                     | 0.42              |
| 23:DB:2723:C:H2'   | 23:DB:2724:U:O4'   | 2.20                     | 0.42              |
| 25:DC:68:ARG:NE    | 25:DC:128:THR:HG23 | 2.34                     | 0.42              |
| 25:DC:93:VAL:HG21  | 25:DC:103:ILE:HG13 | 2.00                     | 0.42              |
| 25:DC:107:LYS:CG   | 25:DC:194:VAL:HG11 | 2.50                     | 0.42              |
| 25:DC:241:LYS:HB3  | 25:DC:243:PRO:HD3  | 2.02                     | 0.42              |
| 26:DD:156:PHE:O    | 26:DD:157:LYS:C    | 2.61                     | 0.42              |
| 27:DE:126:VAL:HG21 | 27:DE:132:LYS:HZ2  | 1.82                     | 0.42              |
| 28:DF:92:GLY:O     | 28:DF:95:MET:HG2   | 2.19                     | 0.42              |
| 31:DJ:35:ARG:NE    | 31:DJ:35:ARG:HA    | 2.35                     | 0.42              |
| 31:DJ:61:LYS:HE2   | 31:DJ:69:ARG:HH22  | 1.84                     | 0.42              |
| 31:DJ:84:ILE:CD1   | 31:DJ:85:LYS:N     | 2.73                     | 0.42              |
| 31:DJ:135:GLN:HE21 | 31:DJ:138:GLN:N    | 2.14                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:DN:37:THR:CG2  | 35:DN:39:PRO:HD2   | 2.41                     | 0.42              |
| 36:DO:25:ARG:HH21 | 36:DO:94:ARG:NH1   | 2.17                     | 0.42              |
| 36:DO:38:GLN:O    | 36:DO:40:ILE:HD13  | 2.18                     | 0.42              |
| 37:DP:105:LYS:HB3 | 37:DP:105:LYS:HE2  | 1.81                     | 0.42              |
| 41:DT:11:LEU:HB2  | 41:DT:12:ARG:H     | 1.59                     | 0.42              |
| 41:DT:69:ARG:HG2  | 41:DT:69:ARG:HH11  | 1.85                     | 0.42              |
| 42:DU:29:SER:O    | 42:DU:30:SER:HB2   | 2.19                     | 0.42              |
| 49:D2:21:ARG:HG3  | 49:D2:31:LEU:CD1   | 2.46                     | 0.42              |
| 49:D2:33:ARG:O    | 49:D2:37:LYS:HB3   | 2.20                     | 0.42              |
| 52:DI:129:GLU:O   | 52:DI:133:ARG:HG3  | 2.19                     | 0.42              |
| 1:AA:41:G:H2'     | 1:AA:42:G:C8       | 2.54                     | 0.42              |
| 1:AA:302:G:H2'    | 1:AA:303:A:H8      | 1.83                     | 0.42              |
| 1:AA:838:G:H2'    | 1:AA:839:C:O4'     | 2.20                     | 0.42              |
| 1:AA:868:C:H2'    | 1:AA:869:G:O4'     | 2.20                     | 0.42              |
| 1:AA:1299:A:N6    | 1:AA:1302:C:H5     | 2.15                     | 0.42              |
| 1:AA:1490:U:H3'   | 1:AA:1491:G:H8     | 1.85                     | 0.42              |
| 2:AC:54:ILE:O     | 2:AC:54:ILE:HG23   | 2.19                     | 0.42              |
| 2:AC:120:THR:HA   | 2:AC:123:LEU:HD12  | 2.01                     | 0.42              |
| 3:AD:63:ILE:C     | 3:AD:65:GLY:H      | 2.27                     | 0.42              |
| 6:AG:114:SER:O    | 6:AG:118:ARG:HG3   | 2.18                     | 0.42              |
| 8:AI:24:ASN:HA    | 8:AI:26:LYS:NZ     | 2.34                     | 0.42              |
| 9:AJ:16:ARG:C     | 9:AJ:17:LEU:HD22   | 2.44                     | 0.42              |
| 9:AJ:48:ARG:HB3   | 9:AJ:66:GLU:HB3    | 2.02                     | 0.42              |
| 10:AK:52:ARG:O    | 10:AK:54:SER:N     | 2.51                     | 0.42              |
| 11:AL:58:ASN:HD22 | 11:AL:58:ASN:C     | 2.26                     | 0.42              |
| 16:AQ:17:GLU:O    | 16:AQ:18:LYS:HB2   | 2.18                     | 0.42              |
| 19:AT:60:GLN:CD   | 19:AT:60:GLN:N     | 2.77                     | 0.42              |
| 20:AB:133:ALA:O   | 20:AB:137:THR:HG23 | 2.20                     | 0.42              |
| 22:BA:54:G:H2'    | 22:BA:55:U:H6      | 1.83                     | 0.42              |
| 23:BB:63:A:H8     | 23:BB:63:A:OP2     | 2.03                     | 0.42              |
| 23:BB:64:A:H2'    | 23:BB:65:U:H6      | 1.80                     | 0.42              |
| 23:BB:649:G:H2'   | 23:BB:650:C:C6     | 2.55                     | 0.42              |
| 23:BB:723:C:H2'   | 23:BB:724:U:C6     | 2.55                     | 0.42              |
| 23:BB:1250:G:C5'  | 38:BQ:5:ARG:HG2    | 2.49                     | 0.42              |
| 23:BB:2080:A:OP1  | 46:BZ:18:CYS:HB2   | 2.20                     | 0.42              |
| 23:BB:2223:G:C2'  | 23:BB:2224:G:H5'   | 2.50                     | 0.42              |
| 23:BB:2286:G:N3   | 23:BB:2286:G:H3'   | 2.34                     | 0.42              |
| 23:BB:2787:C:O2'  | 23:BB:2788:C:H5'   | 2.19                     | 0.42              |
| 23:BB:2840:C:C2   | 23:BB:2841:C:C5    | 3.07                     | 0.42              |
| 24:BV:2:PHE:HE2   | 24:BV:55:GLU:HB3   | 1.84                     | 0.42              |
| 24:BV:6:ALA:HB1   | 24:BV:41:GLU:O     | 2.19                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:BV:80:HIS:HB2   | 24:BV:85:LYS:HG3   | 2.01                     | 0.42              |
| 25:BC:31:PRO:O     | 25:BC:32:LEU:O     | 2.37                     | 0.42              |
| 25:BC:247:TRP:C    | 25:BC:247:TRP:CD1  | 2.98                     | 0.42              |
| 26:BD:1:MET:HB3    | 26:BD:84:LEU:HB2   | 2.00                     | 0.42              |
| 26:BD:149:ASN:ND2  | 26:BD:150:GLN:CD   | 2.78                     | 0.42              |
| 27:BE:195:GLN:H    | 27:BE:199:MET:CA   | 2.28                     | 0.42              |
| 29:BG:51:PHE:CD2   | 29:BG:64:ALA:HA    | 2.54                     | 0.42              |
| 29:BG:104:LEU:HB3  | 29:BG:106:LEU:CD1  | 2.49                     | 0.42              |
| 31:BJ:3:THR:HG21   | 38:BQ:93:ILE:CG1   | 2.40                     | 0.42              |
| 31:BJ:93:ILE:HD13  | 31:BJ:100:VAL:HG11 | 2.01                     | 0.42              |
| 32:BK:34:GLY:O     | 32:BK:35:VAL:C     | 2.63                     | 0.42              |
| 32:BK:38:ILE:HD13  | 32:BK:61:VAL:HG12  | 2.00                     | 0.42              |
| 32:BK:76:VAL:HG12  | 32:BK:77:ILE:N     | 2.35                     | 0.42              |
| 32:BK:80:ASP:OD1   | 37:BP:71:ARG:HG2   | 2.19                     | 0.42              |
| 34:BM:11:LYS:N     | 34:BM:11:LYS:HD3   | 2.34                     | 0.42              |
| 34:BM:45:GLN:NE2   | 34:BM:119:LEU:C    | 2.77                     | 0.42              |
| 35:BN:116:VAL:C    | 35:BN:118:ARG:H    | 2.27                     | 0.42              |
| 36:BO:41:ALA:CB    | 36:BO:45:SER:HB3   | 2.49                     | 0.42              |
| 36:BO:59:ALA:CB    | 36:BO:63:LYS:HE2   | 2.50                     | 0.42              |
| 38:BQ:32:ARG:HD2   | 38:BQ:32:ARG:C     | 2.44                     | 0.42              |
| 41:BT:15:HIS:HB2   | 41:BT:31:VAL:CG2   | 2.50                     | 0.42              |
| 42:BU:54:PRO:CG    | 42:BU:55:GLY:H     | 2.30                     | 0.42              |
| 47:B0:8:THR:HG23   | 47:B0:9:ARG:N      | 2.26                     | 0.42              |
| 1:CA:75:G:H2'      | 1:CA:76:G:O4'      | 2.19                     | 0.42              |
| 1:CA:738:C:H2'     | 1:CA:739:C:C6      | 2.55                     | 0.42              |
| 1:CA:926:G:H5'     | 1:CA:927:G:C5'     | 2.49                     | 0.42              |
| 1:CA:997:U:H2'     | 1:CA:998:C:H6      | 1.79                     | 0.42              |
| 1:CA:1217:C:O2'    | 1:CA:1218:C:H5'    | 2.20                     | 0.42              |
| 2:CC:128:MET:SD    | 2:CC:132:ALA:N     | 2.92                     | 0.42              |
| 3:CD:10:LEU:HD22   | 3:CD:62:ARG:CZ     | 2.49                     | 0.42              |
| 4:CE:52:ALA:HB3    | 4:CE:58:ALA:HB2    | 2.01                     | 0.42              |
| 6:CG:60:ALA:O      | 6:CG:64:ALA:HB3    | 2.19                     | 0.42              |
| 7:CH:72:GLU:N      | 7:CH:129:ALA:HB2   | 2.27                     | 0.42              |
| 9:CJ:18:ILE:HD13   | 9:CJ:72:ARG:HG2    | 2.00                     | 0.42              |
| 14:CO:63:ARG:NH2   | 14:CO:87:ARG:NH1   | 2.67                     | 0.42              |
| 15:CP:54:LEU:CD1   | 15:CP:80:LYS:HG2   | 2.50                     | 0.42              |
| 18:CS:73:PHE:CD1   | 18:CS:73:PHE:N     | 2.88                     | 0.42              |
| 20:CB:99:MET:CA    | 20:CB:106:VAL:HG21 | 2.47                     | 0.42              |
| 20:CB:163:ILE:HD11 | 20:CB:209:VAL:HG11 | 2.01                     | 0.42              |
| 22:DA:45:A:O4'     | 28:DF:91:ARG:CZ    | 2.67                     | 0.42              |
| 23:DB:361:G:H2'    | 23:DB:362:A:C8     | 2.51                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:448:U:H3'   | 27:DE:79:ARG:CZ    | 2.49                     | 0.42              |
| 23:DB:975:A:N3    | 23:DB:975:A:H2'    | 2.35                     | 0.42              |
| 23:DB:1039:A:H2'  | 23:DB:1040:A:C8    | 2.53                     | 0.42              |
| 23:DB:1298:C:O2'  | 23:DB:1301:A:O2'   | 2.36                     | 0.42              |
| 23:DB:1667:G:OP1  | 32:DK:6:THR:HA     | 2.20                     | 0.42              |
| 23:DB:1683:U:O2'  | 23:DB:1684:G:H5'   | 2.19                     | 0.42              |
| 23:DB:1765:U:O2'  | 23:DB:1766:G:H5'   | 2.19                     | 0.42              |
| 23:DB:2047:C:H2'  | 23:DB:2048:G:C8    | 2.52                     | 0.42              |
| 23:DB:2267:A:H3'  | 23:DB:2267:A:N3    | 2.34                     | 0.42              |
| 23:DB:2543:G:H2'  | 23:DB:2544:G:O4'   | 2.20                     | 0.42              |
| 23:DB:2572:A:OP2  | 26:DD:149:ASN:HB3  | 2.19                     | 0.42              |
| 23:DB:2733:A:H8   | 23:DB:2733:A:O5'   | 2.03                     | 0.42              |
| 25:DC:175:LEU:H   | 25:DC:175:LEU:HG   | 1.67                     | 0.42              |
| 25:DC:253:GLY:H   | 25:DC:254:LYS:HE3  | 1.83                     | 0.42              |
| 25:DC:265:PHE:O   | 25:DC:266:ILE:HG12 | 2.20                     | 0.42              |
| 28:DF:41:GLU:C    | 28:DF:43:ILE:N     | 2.77                     | 0.42              |
| 29:DG:16:VAL:HG12 | 29:DG:17:LYS:H     | 1.84                     | 0.42              |
| 29:DG:124:CYS:HB3 | 29:DG:130:ILE:CD1  | 2.49                     | 0.42              |
| 29:DG:124:CYS:C   | 29:DG:126:THR:N    | 2.76                     | 0.42              |
| 29:DG:171:LYS:HZ3 | 29:DG:174:LYS:HD2  | 1.85                     | 0.42              |
| 30:DH:54:LEU:HD23 | 30:DH:57:LYS:CD    | 2.48                     | 0.42              |
| 30:DH:103:VAL:O   | 30:DH:106:ALA:HB3  | 2.20                     | 0.42              |
| 30:DH:129:GLU:H   | 30:DH:129:GLU:HG3  | 1.57                     | 0.42              |
| 31:DJ:69:ARG:HG3  | 31:DJ:69:ARG:NH1   | 2.31                     | 0.42              |
| 32:DK:15:GLY:CA   | 32:DK:52:VAL:HB    | 2.49                     | 0.42              |
| 32:DK:78:ARG:CG   | 37:DP:72:VAL:HG21  | 2.18                     | 0.42              |
| 33:DL:4:ASN:C     | 33:DL:6:LEU:H      | 2.27                     | 0.42              |
| 33:DL:124:GLY:H   | 33:DL:142:ILE:HG13 | 1.85                     | 0.42              |
| 36:DO:67:ASN:HD22 | 36:DO:68:LYS:H     | 1.68                     | 0.42              |
| 36:DO:94:ARG:HG2  | 36:DO:94:ARG:HH11  | 1.84                     | 0.42              |
| 37:DP:94:ALA:C    | 37:DP:96:LEU:H     | 2.27                     | 0.42              |
| 38:DQ:17:LEU:HD12 | 38:DQ:17:LEU:HA    | 1.89                     | 0.42              |
| 38:DQ:50:ARG:NH1  | 38:DQ:53:LYS:HE3   | 2.34                     | 0.42              |
| 38:DQ:94:LEU:O    | 38:DQ:98:ALA:N     | 2.49                     | 0.42              |
| 39:DR:65:ALA:N    | 39:DR:100:GLY:HA2  | 2.34                     | 0.42              |
| 41:DT:6:ARG:O     | 41:DT:8:LEU:N      | 2.52                     | 0.42              |
| 41:DT:84:TYR:O    | 41:DT:85:VAL:C     | 2.63                     | 0.42              |
| 42:DU:42:LYS:H    | 42:DU:57:ILE:CG2   | 2.32                     | 0.42              |
| 47:D0:11:LYS:HD3  | 47:D0:11:LYS:HA    | 1.90                     | 0.42              |
| 47:D0:42:ILE:HG21 | 47:D0:45:ASP:OD2   | 2.19                     | 0.42              |
| 48:D1:40:PRO:O    | 48:D1:41:VAL:C     | 2.63                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 49:D2:39:ARG:HD2  | 49:D2:39:ARG:N    | 2.35                     | 0.42              |
| 52:DI:37:PHE:HB2  | 52:DI:66:PHE:CE2  | 2.55                     | 0.42              |
| 1:AA:278:G:H21    | 1:AA:279:A:N6     | 2.10                     | 0.42              |
| 1:AA:512:U:O2'    | 1:AA:513:C:H5'    | 2.19                     | 0.42              |
| 1:AA:529:G:O6     | 11:AL:45:ASN:HA   | 2.19                     | 0.42              |
| 1:AA:687:A:C2     | 1:AA:704:A:C6     | 3.07                     | 0.42              |
| 1:AA:908:A:O2'    | 1:AA:909:A:H5'    | 2.19                     | 0.42              |
| 1:AA:958:A:C4'    | 18:AS:54:ARG:HH21 | 2.33                     | 0.42              |
| 1:AA:1101:A:O2'   | 1:AA:1102:A:O4'   | 2.27                     | 0.42              |
| 1:AA:1432:G:O2'   | 1:AA:1468:A:N6    | 2.50                     | 0.42              |
| 1:AA:1447:A:H5'   | 1:AA:1448:C:H5    | 1.85                     | 0.42              |
| 1:AA:1521:C:H2'   | 1:AA:1522:U:H6    | 1.84                     | 0.42              |
| 3:AD:54:LEU:C     | 3:AD:57:LYS:HB3   | 2.45                     | 0.42              |
| 6:AG:20:GLU:O     | 6:AG:23:ALA:HB3   | 2.19                     | 0.42              |
| 7:AH:83:ARG:NH1   | 7:AH:123:GLU:OE1  | 2.53                     | 0.42              |
| 9:AJ:25:ILE:HG23  | 9:AJ:29:ALA:CB    | 2.47                     | 0.42              |
| 10:AK:70:ALA:HA   | 10:AK:74:LYS:HD3  | 2.01                     | 0.42              |
| 11:AL:43:LYS:N    | 11:AL:44:PRO:CD   | 2.81                     | 0.42              |
| 12:AM:10:ASP:HA   | 12:AM:44:ILE:HD11 | 2.01                     | 0.42              |
| 12:AM:23:GLY:CA   | 12:AM:64:VAL:HG13 | 2.43                     | 0.42              |
| 16:AQ:7:LEU:HB2   | 16:AQ:60:ILE:HG12 | 2.02                     | 0.42              |
| 16:AQ:30:HIS:N    | 16:AQ:35:LYS:H    | 2.17                     | 0.42              |
| 20:AB:15:PHE:HD1  | 20:AB:16:GLY:N    | 2.18                     | 0.42              |
| 23:BB:26:G:C2'    | 23:BB:27:G:O4'    | 2.67                     | 0.42              |
| 23:BB:181:A:O2'   | 23:BB:182:A:H5'   | 2.19                     | 0.42              |
| 23:BB:678:C:H2'   | 23:BB:679:C:C6    | 2.53                     | 0.42              |
| 23:BB:775:G:C5    | 23:BB:794:A:C8    | 3.08                     | 0.42              |
| 23:BB:1068:G:C6   | 23:BB:1069:A:N6   | 2.87                     | 0.42              |
| 23:BB:1156:A:C5   | 38:BQ:47:ARG:NH1  | 2.88                     | 0.42              |
| 23:BB:1403:A:H2'  | 23:BB:1404:C:C6   | 2.54                     | 0.42              |
| 23:BB:1637:A:H5'  | 23:BB:1760:C:O2'  | 2.20                     | 0.42              |
| 23:BB:1713:A:N6   | 23:BB:1745:A:H61  | 2.18                     | 0.42              |
| 23:BB:1841:U:C2   | 23:BB:1842:G:C8   | 3.07                     | 0.42              |
| 23:BB:2347:C:OP1  | 23:BB:2347:C:H4'  | 2.19                     | 0.42              |
| 23:BB:2540:C:O2'  | 23:BB:2541:A:H5'  | 2.20                     | 0.42              |
| 23:BB:2686:G:H2'  | 23:BB:2687:U:C6   | 2.54                     | 0.42              |
| 23:BB:2723:C:H2'  | 23:BB:2724:U:O4'  | 2.20                     | 0.42              |
| 26:BD:88:GLU:C    | 26:BD:90:PHE:H    | 2.28                     | 0.42              |
| 26:BD:175:LEU:CD2 | 26:BD:190:LYS:HB3 | 2.50                     | 0.42              |
| 31:BJ:41:LYS:HE3  | 31:BJ:42:ALA:C    | 2.45                     | 0.42              |
| 33:BL:78:ARG:NH1  | 33:BL:80:SER:N    | 2.68                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:BM:69:PRO:HA   | 34:BM:93:VAL:HB    | 2.01                     | 0.42              |
| 38:BQ:3:VAL:O     | 38:BQ:4:LYS:C      | 2.62                     | 0.42              |
| 39:BR:21:ARG:HH11 | 39:BR:21:ARG:HG2   | 1.84                     | 0.42              |
| 40:BS:29:VAL:HG21 | 40:BS:70:LYS:N     | 2.35                     | 0.42              |
| 40:BS:50:VAL:HG21 | 40:BS:103:ILE:CG2  | 2.50                     | 0.42              |
| 40:BS:82:MET:HB2  | 40:BS:98:LYS:CG    | 2.50                     | 0.42              |
| 42:BU:4:ILE:HG21  | 42:BU:25:LYS:HZ3   | 1.84                     | 0.42              |
| 42:BU:33:VAL:HG12 | 42:BU:35:VAL:HG23  | 2.02                     | 0.42              |
| 42:BU:90:LYS:HD2  | 42:BU:91:LYS:N     | 2.34                     | 0.42              |
| 43:BW:35:ILE:HG13 | 43:BW:36:ILE:N     | 2.33                     | 0.42              |
| 44:BX:44:LYS:HD2  | 44:BX:44:LYS:C     | 2.45                     | 0.42              |
| 46:BZ:15:SER:HB3  | 46:BZ:23:LYS:HE2   | 2.02                     | 0.42              |
| 1:CA:41:G:H2'     | 1:CA:42:G:C8       | 2.54                     | 0.42              |
| 1:CA:69:G:H2'     | 1:CA:70:U:C6       | 2.55                     | 0.42              |
| 1:CA:109:A:N1     | 1:CA:326:G:C6      | 2.88                     | 0.42              |
| 1:CA:327:A:O2'    | 1:CA:328:C:O4'     | 2.33                     | 0.42              |
| 1:CA:404:G:H2'    | 1:CA:405:U:H6      | 1.85                     | 0.42              |
| 1:CA:429:U:H4'    | 1:CA:430:A:O5'     | 2.16                     | 0.42              |
| 1:CA:538:G:H2'    | 1:CA:539:A:C8      | 2.54                     | 0.42              |
| 1:CA:896:C:O2'    | 1:CA:897:C:H5'     | 2.19                     | 0.42              |
| 1:CA:1014:A:H2'   | 1:CA:1015:G:C8     | 2.54                     | 0.42              |
| 1:CA:1082:A:H2'   | 1:CA:1083:U:O4'    | 2.20                     | 0.42              |
| 1:CA:1200:C:OP1   | 1:CA:1201:A:H3'    | 2.20                     | 0.42              |
| 2:CC:110:LEU:HD13 | 2:CC:143:LEU:CD2   | 2.50                     | 0.42              |
| 3:CD:195:ASN:HB2  | 3:CD:198:LEU:HD12  | 2.02                     | 0.42              |
| 5:CF:29:ILE:HG21  | 5:CF:64:VAL:CG1    | 2.49                     | 0.42              |
| 7:CH:65:PHE:CD2   | 7:CH:66:GLN:HG2    | 2.55                     | 0.42              |
| 12:CM:70:ARG:NH1  | 28:DF:135:ILE:HD13 | 2.35                     | 0.42              |
| 12:CM:78:ARG:HD2  | 12:CM:79:LEU:N     | 2.35                     | 0.42              |
| 14:CO:87:ARG:O    | 14:CO:87:ARG:HG3   | 2.20                     | 0.42              |
| 15:CP:10:GLY:HA3  | 15:CP:15:PRO:HA    | 2.01                     | 0.42              |
| 15:CP:26:ASN:ND2  | 15:CP:31:ARG:HB3   | 2.34                     | 0.42              |
| 23:DB:164:C:H2'   | 23:DB:165:A:H5'    | 2.01                     | 0.42              |
| 23:DB:249:C:O2'   | 50:D3:7:ARG:NE     | 2.52                     | 0.42              |
| 23:DB:506:G:H1'   | 23:DB:507:A:C8     | 2.54                     | 0.42              |
| 23:DB:647:G:H2'   | 23:DB:648:G:C8     | 2.55                     | 0.42              |
| 23:DB:686:U:O2'   | 49:D2:5:PHE:O      | 2.34                     | 0.42              |
| 23:DB:795:C:H2'   | 23:DB:796:C:C6     | 2.55                     | 0.42              |
| 23:DB:906:U:H4'   | 34:DM:26:VAL:CG1   | 2.49                     | 0.42              |
| 23:DB:982:C:O2    | 23:DB:982:C:H2'    | 2.20                     | 0.42              |
| 23:DB:1029:A:H3'  | 23:DB:1030:C:C6    | 2.53                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:1264:A:H5'   | 47:D0:7:PRO:HG3    | 2.01                     | 0.42              |
| 23:DB:1372:U:H2'   | 23:DB:1373:A:C8    | 2.55                     | 0.42              |
| 23:DB:1773:A:H2'   | 23:DB:1774:C:O4'   | 2.19                     | 0.42              |
| 23:DB:2135:A:N3    | 23:DB:2135:A:H2'   | 2.35                     | 0.42              |
| 23:DB:2282:G:H5''  | 23:DB:2283:C:O4'   | 2.20                     | 0.42              |
| 23:DB:2425:A:H4'   | 23:DB:2426:A:OP2   | 2.19                     | 0.42              |
| 23:DB:2540:C:O2'   | 23:DB:2541:A:H5'   | 2.20                     | 0.42              |
| 24:DV:23:ALA:O     | 24:DV:24:ASN:HB2   | 2.19                     | 0.42              |
| 25:DC:8:THR:O      | 25:DC:10:PRO:HD3   | 2.20                     | 0.42              |
| 25:DC:21:PRO:N     | 25:DC:202:ARG:HH11 | 2.18                     | 0.42              |
| 25:DC:42:ARG:HE    | 25:DC:43:ASN:H     | 1.68                     | 0.42              |
| 25:DC:110:LYS:HE3  | 25:DC:110:LYS:CA   | 2.49                     | 0.42              |
| 25:DC:222:THR:OG1  | 25:DC:223:ALA:N    | 2.53                     | 0.42              |
| 26:DD:7:LYS:HA     | 26:DD:26:VAL:HA    | 2.01                     | 0.42              |
| 26:DD:46:ARG:N     | 26:DD:82:PHE:HA    | 2.35                     | 0.42              |
| 27:DE:175:ILE:CG2  | 27:DE:180:LEU:HD11 | 2.49                     | 0.42              |
| 28:DF:65:LEU:O     | 28:DF:66:ILE:HB    | 2.20                     | 0.42              |
| 28:DF:71:LYS:HE2   | 28:DF:72:SER:C     | 2.45                     | 0.42              |
| 28:DF:111:ARG:HH11 | 28:DF:111:ARG:HG2  | 1.85                     | 0.42              |
| 29:DG:4:ALA:HA     | 29:DG:68:ARG:HH22  | 1.85                     | 0.42              |
| 29:DG:36:LEU:HB2   | 29:DG:40:VAL:HG11  | 2.02                     | 0.42              |
| 29:DG:43:LYS:HB3   | 29:DG:44:HIS:H     | 1.71                     | 0.42              |
| 31:DJ:74:TYR:OH    | 31:DJ:100:VAL:HG23 | 2.20                     | 0.42              |
| 35:DN:67:PHE:O     | 35:DN:71:ARG:HA    | 2.20                     | 0.42              |
| 36:DO:109:ALA:HA   | 36:DO:112:GLU:CD   | 2.45                     | 0.42              |
| 37:DP:46:VAL:HB    | 37:DP:65:ASN:OD1   | 2.19                     | 0.42              |
| 37:DP:100:ARG:HB3  | 37:DP:100:ARG:NH1  | 2.14                     | 0.42              |
| 37:DP:105:LYS:C    | 37:DP:107:ALA:H    | 2.28                     | 0.42              |
| 38:DQ:77:LYS:O     | 38:DQ:80:ASN:HB3   | 2.19                     | 0.42              |
| 44:DX:16:THR:HG23  | 44:DX:21:LEU:HD12  | 2.00                     | 0.42              |
| 44:DX:37:LEU:HG    | 44:DX:38:GLN:N     | 2.35                     | 0.42              |
| 50:D3:4:LYS:HZ1    | 50:D3:60:CYS:HB3   | 1.85                     | 0.42              |
| 50:D3:44:ARG:HG2   | 50:D3:45:PRO:HD2   | 2.02                     | 0.42              |
| 51:D4:24:ARG:HE    | 51:D4:37:GLN:HA    | 1.84                     | 0.42              |
| 52:DI:121:ILE:HD11 | 52:DI:122:GLU:OE2  | 2.20                     | 0.42              |
| 1:AA:162:A:H2'     | 1:AA:163:C:O4'     | 2.20                     | 0.42              |
| 1:AA:545:C:H5''    | 3:AD:68:GLU:HG2    | 2.00                     | 0.42              |
| 1:AA:734:G:O2'     | 17:AR:59:LYS:HD3   | 2.19                     | 0.42              |
| 1:AA:806:C:O2'     | 1:AA:807:A:H5'     | 2.19                     | 0.42              |
| 1:AA:829:G:H4'     | 20:AB:24:PRO:HG3   | 2.02                     | 0.42              |
| 1:AA:896:C:O2'     | 1:AA:897:C:H5'     | 2.19                     | 0.42              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:1096:C:O2'   | 1:AA:1097:C:H5'   | 2.20                     | 0.42              |
| 1:AA:1111:A:H2    | 2:AC:176:THR:HG23 | 1.85                     | 0.42              |
| 1:AA:1286:U:N1    | 1:AA:1286:U:O5'   | 2.52                     | 0.42              |
| 1:AA:1389:C:H2'   | 1:AA:1390:U:C6    | 2.55                     | 0.42              |
| 2:AC:84:GLU:HA    | 2:AC:87:ARG:NH2   | 2.35                     | 0.42              |
| 6:AG:14:ASP:O     | 6:AG:18:GLY:HA2   | 2.19                     | 0.42              |
| 15:AP:45:GLU:C    | 15:AP:47:GLU:H    | 2.28                     | 0.42              |
| 19:AT:50:PHE:O    | 19:AT:53:MET:HE3  | 2.20                     | 0.42              |
| 20:AB:20:ARG:HG3  | 20:AB:20:ARG:NH1  | 2.33                     | 0.42              |
| 22:BA:50:A:H5''   | 36:BO:68:LYS:CG   | 2.49                     | 0.42              |
| 23:BB:159:G:O2'   | 23:BB:160:A:H5''  | 2.20                     | 0.42              |
| 23:BB:319:G:H2'   | 23:BB:320:A:C8    | 2.55                     | 0.42              |
| 23:BB:651:G:C5'   | 50:B3:17:GLY:HA3  | 2.50                     | 0.42              |
| 23:BB:724:U:H2'   | 23:BB:725:G:O4'   | 2.19                     | 0.42              |
| 23:BB:948:C:H2'   | 23:BB:949:G:C8    | 2.53                     | 0.42              |
| 23:BB:1156:A:H62  | 38:BQ:47:ARG:HD3  | 1.85                     | 0.42              |
| 23:BB:1255:U:C2'  | 27:BE:67:ARG:HB3  | 2.50                     | 0.42              |
| 23:BB:1322:A:C5   | 23:BB:1323:C:C5   | 3.08                     | 0.42              |
| 23:BB:1390:U:O2'  | 23:BB:1391:U:H5'  | 2.20                     | 0.42              |
| 23:BB:1616:A:H4'  | 23:BB:1617:C:OP2  | 2.19                     | 0.42              |
| 23:BB:1791:A:C2   | 23:BB:1829:A:O4'  | 2.73                     | 0.42              |
| 23:BB:1987:A:H2'  | 23:BB:1988:G:C8   | 2.54                     | 0.42              |
| 23:BB:2019:A:C6   | 23:BB:2020:A:N7   | 2.88                     | 0.42              |
| 23:BB:2228:G:OP1  | 25:BC:257:ARG:HB2 | 2.20                     | 0.42              |
| 23:BB:2543:G:H2'  | 23:BB:2544:G:O4'  | 2.20                     | 0.42              |
| 23:BB:2728:U:H5'  | 32:BK:70:ARG:NH2  | 2.34                     | 0.42              |
| 24:BV:4:ILE:N     | 24:BV:62:THR:O    | 2.52                     | 0.42              |
| 24:BV:66:ASP:O    | 24:BV:66:ASP:OD1  | 2.37                     | 0.42              |
| 25:BC:225:ASN:N   | 25:BC:226:PRO:HD3 | 2.35                     | 0.42              |
| 25:BC:251:THR:O   | 25:BC:252:LYS:HB2 | 2.19                     | 0.42              |
| 26:BD:170:VAL:O   | 26:BD:171:THR:HB  | 2.19                     | 0.42              |
| 27:BE:43:THR:HG23 | 27:BE:44:ARG:CZ   | 2.50                     | 0.42              |
| 27:BE:77:ILE:HB   | 27:BE:78:TRP:CE3  | 2.54                     | 0.42              |
| 28:BF:163:GLU:C   | 28:BF:165:GLY:N   | 2.77                     | 0.42              |
| 30:BH:3:VAL:HG22  | 30:BH:21:VAL:CG1  | 2.45                     | 0.42              |
| 31:BJ:35:ARG:HH21 | 31:BJ:40:HIS:H    | 1.66                     | 0.42              |
| 33:BL:69:ARG:O    | 33:BL:69:ARG:HG3  | 2.19                     | 0.42              |
| 34:BM:17:ASN:HB3  | 34:BM:18:ARG:H    | 1.49                     | 0.42              |
| 36:BO:54:VAL:O    | 36:BO:55:GLU:C    | 2.62                     | 0.42              |
| 37:BP:15:ASP:C    | 37:BP:17:PRO:HD3  | 2.45                     | 0.42              |
| 37:BP:18:SER:HB2  | 37:BP:87:ARG:CZ   | 2.50                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:BQ:108:LEU:HD22 | 39:BR:52:PRO:HA    | 2.00                     | 0.42              |
| 42:BU:84:PHE:HD2   | 42:BU:87:GLU:HB2   | 1.84                     | 0.42              |
| 48:B1:7:LYS:O      | 48:B1:7:LYS:HG3    | 2.20                     | 0.42              |
| 49:B2:13:ASN:CB    | 49:B2:18:PHE:HD2   | 2.29                     | 0.42              |
| 1:CA:234:C:H2'     | 1:CA:235:C:H6      | 1.84                     | 0.42              |
| 1:CA:393:A:O2'     | 1:CA:394:G:H5'     | 2.20                     | 0.42              |
| 1:CA:489:C:H2'     | 1:CA:490:C:C6      | 2.54                     | 0.42              |
| 1:CA:925:G:C2      | 1:CA:927:G:C8      | 3.08                     | 0.42              |
| 1:CA:939:G:H2'     | 1:CA:940:C:C6      | 2.54                     | 0.42              |
| 1:CA:939:G:C5'     | 6:CG:101:ARG:HH22  | 2.29                     | 0.42              |
| 2:CC:33:ASP:O      | 2:CC:37:LYS:HG3    | 2.19                     | 0.42              |
| 2:CC:54:ILE:HG23   | 2:CC:54:ILE:O      | 2.20                     | 0.42              |
| 3:CD:142:VAL:HG22  | 3:CD:179:GLY:HA3   | 2.00                     | 0.42              |
| 8:CI:6:TYR:CG      | 8:CI:7:GLY:N       | 2.86                     | 0.42              |
| 9:CJ:68:ARG:HD3    | 9:CJ:70:HIS:NE2    | 2.35                     | 0.42              |
| 12:CM:1:ALA:O      | 12:CM:3:ILE:HG13   | 2.19                     | 0.42              |
| 16:CQ:7:LEU:O      | 16:CQ:59:GLU:HA    | 2.19                     | 0.42              |
| 20:CB:169:HIS:O    | 20:CB:170:ILE:C    | 2.63                     | 0.42              |
| 22:DA:38:C:H2'     | 22:DA:39:A:O4'     | 2.18                     | 0.42              |
| 22:DA:49:C:C5'     | 36:DO:101:GLY:HA3  | 2.50                     | 0.42              |
| 23:DB:340:A:O2'    | 23:DB:341:C:H5'    | 2.20                     | 0.42              |
| 23:DB:396:G:O2'    | 23:DB:397:U:H5'    | 2.20                     | 0.42              |
| 23:DB:414:C:H1'    | 23:DB:1864:U:H1'   | 2.01                     | 0.42              |
| 23:DB:607:U:C4     | 23:DB:620:G:O4'    | 2.73                     | 0.42              |
| 23:DB:748:G:O5'    | 40:DS:89:ALA:HB2   | 2.20                     | 0.42              |
| 23:DB:848:C:H2'    | 23:DB:849:A:H8     | 1.84                     | 0.42              |
| 23:DB:929:U:O2     | 45:DY:25:GLY:HA2   | 2.20                     | 0.42              |
| 23:DB:978:G:O4'    | 23:DB:1001:A:H2    | 2.03                     | 0.42              |
| 23:DB:1080:A:H4'   | 52:DI:126:ARG:CD   | 2.50                     | 0.42              |
| 23:DB:1254:A:C6    | 27:DE:77:ILE:HD12  | 2.55                     | 0.42              |
| 23:DB:1268:A:H2'   | 23:DB:1269:A:H8    | 1.85                     | 0.42              |
| 23:DB:1410:G:H2'   | 23:DB:1411:U:H6    | 1.77                     | 0.42              |
| 23:DB:2065:C:H1'   | 23:DB:2449:U:O2    | 2.20                     | 0.42              |
| 23:DB:2080:A:H5'   | 46:DZ:17:SER:HB2   | 2.00                     | 0.42              |
| 23:DB:2183:A:H8    | 23:DB:2183:A:O5'   | 2.02                     | 0.42              |
| 23:DB:2276:G:N7    | 43:DW:11:ASN:ND2   | 2.66                     | 0.42              |
| 23:DB:2341:G:H2'   | 23:DB:2342:C:H6    | 1.84                     | 0.42              |
| 23:DB:2365:G:H4'   | 43:DW:65:LYS:CD    | 2.49                     | 0.42              |
| 23:DB:2394:C:P     | 33:DL:63:LYS:HD2   | 2.60                     | 0.42              |
| 23:DB:2840:C:C2    | 23:DB:2841:C:C5    | 3.07                     | 0.42              |
| 25:DC:78:GLU:CD    | 25:DC:100:ARG:HH21 | 2.27                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DE:150:THR:HG23 | 27:DE:167:VAL:HG11 | 2.02                     | 0.42              |
| 29:DG:10:VAL:N     | 29:DG:11:PRO:CD    | 2.83                     | 0.42              |
| 33:DL:14:LYS:CD    | 33:DL:15:ALA:N     | 2.83                     | 0.42              |
| 33:DL:118:THR:HG21 | 33:DL:137:ALA:HB3  | 2.00                     | 0.42              |
| 34:DM:31:PHE:O     | 34:DM:102:LEU:HA   | 2.20                     | 0.42              |
| 35:DN:103:ARG:HG2  | 35:DN:106:ASP:CG   | 2.45                     | 0.42              |
| 38:DQ:36:GLN:C     | 38:DQ:38:VAL:H     | 2.27                     | 0.42              |
| 38:DQ:52:ARG:HH11  | 38:DQ:52:ARG:CB    | 2.32                     | 0.42              |
| 40:DS:1:MET:O      | 40:DS:2:GLU:C      | 2.62                     | 0.42              |
| 40:DS:28:LYS:O     | 40:DS:29:VAL:HB    | 2.20                     | 0.42              |
| 41:DT:31:VAL:HG23  | 41:DT:83:ALA:O     | 2.20                     | 0.42              |
| 42:DU:64:ILE:O     | 42:DU:64:ILE:HG22  | 2.19                     | 0.42              |
| 46:DZ:36:VAL:HG12  | 46:DZ:42:PRO:HB2   | 2.01                     | 0.42              |
| 47:D0:28:SER:HB3   | 47:D0:36:LYS:O     | 2.19                     | 0.42              |
| 48:D1:9:LYS:HA     | 48:D1:24:LYS:HB2   | 2.02                     | 0.42              |
| 50:D3:37:THR:HA    | 50:D3:40:LYS:HD3   | 2.02                     | 0.42              |
| 52:DI:100:ILE:HG23 | 52:DI:104:GLN:OE1  | 2.20                     | 0.42              |
| 1:AA:21:G:H1'      | 1:AA:914:A:H61     | 1.84                     | 0.42              |
| 1:AA:257:G:H2'     | 1:AA:258:G:C8      | 2.55                     | 0.42              |
| 1:AA:309:A:O2'     | 1:AA:607:A:N1      | 2.52                     | 0.42              |
| 1:AA:489:C:H2'     | 1:AA:490:C:C6      | 2.55                     | 0.42              |
| 1:AA:771:G:H2'     | 1:AA:772:U:C6      | 2.54                     | 0.42              |
| 1:AA:1073:U:O3'    | 20:AB:104:LYS:NZ   | 2.53                     | 0.42              |
| 1:AA:1091:U:H2'    | 1:AA:1093:A:OP2    | 2.19                     | 0.42              |
| 1:AA:1441:A:H2'    | 1:AA:1442:G:O4'    | 2.20                     | 0.42              |
| 1:AA:1477:U:H2'    | 1:AA:1478:U:H6     | 1.83                     | 0.42              |
| 2:AC:38:VAL:HG12   | 2:AC:93:ILE:HG21   | 2.01                     | 0.42              |
| 3:AD:36:ALA:C      | 3:AD:38:GLY:N      | 2.78                     | 0.42              |
| 4:AE:50:GLY:H      | 4:AE:62:ALA:HB2    | 1.85                     | 0.42              |
| 4:AE:110:MET:SD    | 4:AE:110:MET:N     | 2.92                     | 0.42              |
| 5:AF:77:THR:O      | 5:AF:81:ASN:HB2    | 2.20                     | 0.42              |
| 6:AG:30:MET:SD     | 6:AG:35:LYS:HB2    | 2.59                     | 0.42              |
| 6:AG:148:LYS:HA    | 6:AG:151:ALA:HB3   | 2.02                     | 0.42              |
| 12:AM:14:ALA:CB    | 12:AM:33:LEU:HD11  | 2.50                     | 0.42              |
| 12:AM:84:CYS:HA    | 18:AS:72:GLU:O     | 2.19                     | 0.42              |
| 13:AN:30:ILE:C     | 13:AN:32:ASP:N     | 2.77                     | 0.42              |
| 14:AO:10:ILE:HD13  | 14:AO:30:LEU:HA    | 2.02                     | 0.42              |
| 14:AO:34:GLN:HG2   | 14:AO:58:MET:HE1   | 2.02                     | 0.42              |
| 15:AP:71:VAL:HA    | 15:AP:74:LEU:CD1   | 2.49                     | 0.42              |
| 16:AQ:26:ARG:O     | 16:AQ:38:LYS:HA    | 2.19                     | 0.42              |
| 16:AQ:62:GLU:HG3   | 16:AQ:72:TRP:CH2   | 2.55                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:AS:47:THR:HA    | 18:AS:59:VAL:O     | 2.20                     | 0.42              |
| 20:AB:35:ASN:O     | 20:AB:36:LYS:HB2   | 2.19                     | 0.42              |
| 20:AB:53:LEU:HB3   | 20:AB:219:THR:HG21 | 2.02                     | 0.42              |
| 20:AB:80:LYS:HB3   | 20:AB:90:PHE:CE1   | 2.54                     | 0.42              |
| 21:AU:45:LYS:O     | 21:AU:48:LYS:HG3   | 2.19                     | 0.42              |
| 22:BA:100:G:H5''   | 23:BB:915:C:O2'    | 2.19                     | 0.42              |
| 23:BB:18:U:O3'     | 38:BQ:22:GLY:HA3   | 2.19                     | 0.42              |
| 23:BB:45:G:H5'     | 23:BB:46:G:OP1     | 2.19                     | 0.42              |
| 23:BB:46:G:H2'     | 23:BB:47:C:C6      | 2.55                     | 0.42              |
| 23:BB:100:U:O2'    | 23:BB:101:A:O5'    | 2.38                     | 0.42              |
| 23:BB:288:U:H2'    | 23:BB:289:G:H8     | 1.85                     | 0.42              |
| 23:BB:729:G:H8     | 23:BB:764:A:OP1    | 2.03                     | 0.42              |
| 23:BB:834:G:H2'    | 23:BB:835:C:C6     | 2.54                     | 0.42              |
| 23:BB:1268:A:H2'   | 23:BB:1269:A:H8    | 1.85                     | 0.42              |
| 23:BB:1528:A:C2'   | 23:BB:1529:G:H5'   | 2.50                     | 0.42              |
| 23:BB:1797:G:C5'   | 25:BC:251:THR:HG23 | 2.50                     | 0.42              |
| 23:BB:1820:U:H3    | 25:BC:197:ALA:CB   | 2.33                     | 0.42              |
| 23:BB:2054:A:OP1   | 23:BB:2055:C:H4'   | 2.20                     | 0.42              |
| 23:BB:2299:U:H2'   | 23:BB:2300:C:H6    | 1.85                     | 0.42              |
| 23:BB:2428:G:H5''  | 23:BB:2429:G:O5'   | 2.19                     | 0.42              |
| 23:BB:2733:A:H8    | 23:BB:2733:A:O5'   | 2.03                     | 0.42              |
| 23:BB:2733:A:N1    | 26:BD:209:ALA:O    | 2.53                     | 0.42              |
| 24:BV:44:HIS:CE1   | 24:BV:85:LYS:HB2   | 2.55                     | 0.42              |
| 25:BC:191:LEU:HD13 | 25:BC:191:LEU:O    | 2.20                     | 0.42              |
| 26:BD:29:VAL:HG23  | 26:BD:51:THR:CG2   | 2.50                     | 0.42              |
| 30:BH:6:LEU:H      | 30:BH:16:GLY:N     | 2.17                     | 0.42              |
| 31:BJ:7:LYS:C      | 31:BJ:9:GLU:N      | 2.78                     | 0.42              |
| 31:BJ:120:ARG:O    | 31:BJ:120:ARG:HD3  | 2.20                     | 0.42              |
| 32:BK:24:VAL:HG22  | 32:BK:39:ILE:HD12  | 2.01                     | 0.42              |
| 32:BK:119:ALA:N    | 32:BK:120:PRO:CD   | 2.82                     | 0.42              |
| 33:BL:39:LYS:C     | 33:BL:41:ARG:H     | 2.27                     | 0.42              |
| 33:BL:94:THR:HG23  | 33:BL:95:LEU:N     | 2.34                     | 0.42              |
| 35:BN:36:THR:O     | 35:BN:37:THR:O     | 2.37                     | 0.42              |
| 37:BP:92:ARG:H     | 37:BP:113:LEU:HD23 | 1.84                     | 0.42              |
| 38:BQ:58:GLN:O     | 38:BQ:62:ALA:HB2   | 2.19                     | 0.42              |
| 41:BT:6:ARG:HE     | 41:BT:6:ARG:HB2    | 1.57                     | 0.42              |
| 42:BU:25:LYS:HA    | 42:BU:35:VAL:N     | 2.29                     | 0.42              |
| 42:BU:70:ALA:HB3   | 42:BU:77:GLY:C     | 2.44                     | 0.42              |
| 43:BW:54:ARG:CZ    | 43:BW:54:ARG:HB2   | 2.50                     | 0.42              |
| 44:BX:29:ARG:O     | 44:BX:29:ARG:HG2   | 2.20                     | 0.42              |
| 48:B1:34:GLU:N     | 48:B1:52:LYS:O     | 2.53                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:B3:42:HIS:ND1   | 50:B3:42:HIS:C     | 2.77                     | 0.42              |
| 1:CA:257:G:H2'     | 1:CA:258:G:C8      | 2.55                     | 0.42              |
| 1:CA:297:G:N2      | 1:CA:300:A:OP2     | 2.51                     | 0.42              |
| 1:CA:462:G:H3'     | 1:CA:463:U:C5'     | 2.48                     | 0.42              |
| 1:CA:687:A:C2      | 1:CA:704:A:C6      | 3.08                     | 0.42              |
| 1:CA:716:A:N3      | 10:CK:119:GLY:HA2  | 2.34                     | 0.42              |
| 1:CA:761:G:H2'     | 1:CA:762:U:H6      | 1.84                     | 0.42              |
| 1:CA:771:G:H2'     | 1:CA:772:U:C6      | 2.54                     | 0.42              |
| 2:CC:5:HIS:ND1     | 13:CN:88:MET:HB3   | 2.35                     | 0.42              |
| 2:CC:68:HIS:HA     | 2:CC:103:ALA:HB3   | 2.02                     | 0.42              |
| 3:CD:55:ARG:HA     | 3:CD:55:ARG:HD2    | 1.78                     | 0.42              |
| 3:CD:67:LEU:O      | 3:CD:71:PHE:HB2    | 2.19                     | 0.42              |
| 4:CE:144:GLU:HA    | 4:CE:146:MET:SD    | 2.59                     | 0.42              |
| 6:CG:11:ILE:HG22   | 6:CG:12:LEU:H      | 1.84                     | 0.42              |
| 14:CO:10:ILE:HD13  | 14:CO:30:LEU:HG    | 2.02                     | 0.42              |
| 15:CP:4:ILE:HG22   | 15:CP:19:VAL:HG23  | 2.02                     | 0.42              |
| 15:CP:6:LEU:HB3    | 15:CP:17:TYR:HB3   | 2.01                     | 0.42              |
| 19:CT:67:HIS:O     | 19:CT:70:LYS:HG2   | 2.19                     | 0.42              |
| 20:CB:26:MET:HE1   | 20:CB:186:VAL:CB   | 2.47                     | 0.42              |
| 20:CB:163:ILE:CG2  | 20:CB:164:ASP:H    | 2.25                     | 0.42              |
| 20:CB:202:ASN:HD22 | 20:CB:203:ASP:N    | 2.12                     | 0.42              |
| 23:DB:86:G:P       | 42:DU:28:LEU:HD22  | 2.60                     | 0.42              |
| 23:DB:265:A:H2'    | 23:DB:266:G:C1'    | 2.50                     | 0.42              |
| 23:DB:357:C:H2'    | 23:DB:358:U:C6     | 2.54                     | 0.42              |
| 23:DB:705:A:N6     | 23:DB:726:G:H1'    | 2.35                     | 0.42              |
| 23:DB:795:C:H2'    | 23:DB:796:C:H6     | 1.84                     | 0.42              |
| 23:DB:822:G:H2'    | 23:DB:823:C:H6     | 1.84                     | 0.42              |
| 23:DB:876:C:H5'    | 23:DB:877:A:OP2    | 2.20                     | 0.42              |
| 23:DB:963:U:H5''   | 55:DB:3696:HOH:O   | 2.19                     | 0.42              |
| 23:DB:1161:C:H2'   | 23:DB:1162:G:C8    | 2.53                     | 0.42              |
| 23:DB:1289:C:C2    | 23:DB:1290:C:C5    | 3.07                     | 0.42              |
| 23:DB:1463:C:H2'   | 23:DB:1464:G:H8    | 1.82                     | 0.42              |
| 23:DB:2077:A:N6    | 23:DB:2435:A:N6    | 2.68                     | 0.42              |
| 23:DB:2617:U:C4    | 23:DB:2618:G:N7    | 2.87                     | 0.42              |
| 25:DC:179:GLU:OE2  | 25:DC:266:ILE:HA   | 2.19                     | 0.42              |
| 26:DD:77:ARG:NH2   | 26:DD:79:LEU:HB2   | 2.14                     | 0.42              |
| 26:DD:118:PHE:CA   | 26:DD:164:GLN:HG2  | 2.50                     | 0.42              |
| 26:DD:122:VAL:HB   | 26:DD:141:ARG:NH1  | 2.35                     | 0.42              |
| 26:DD:156:PHE:CG   | 31:DJ:81:ILE:HG21  | 2.54                     | 0.42              |
| 26:DD:199:SER:O    | 26:DD:201:LEU:HD13 | 2.20                     | 0.42              |
| 27:DE:148:ILE:HD12 | 27:DE:148:ILE:C    | 2.45                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:DE:188:MET:SD  | 27:DE:188:MET:C    | 3.03                     | 0.42              |
| 28:DF:7:TYR:C     | 28:DF:11:VAL:HB    | 2.45                     | 0.42              |
| 29:DG:3:VAL:CG2   | 29:DG:4:ALA:N      | 2.83                     | 0.42              |
| 29:DG:29:ASN:HB2  | 29:DG:78:VAL:HA    | 2.01                     | 0.42              |
| 29:DG:41:GLU:CD   | 29:DG:54:ARG:HA    | 2.45                     | 0.42              |
| 30:DH:8:LYS:HD2   | 30:DH:14:SER:HA    | 2.02                     | 0.42              |
| 31:DJ:107:GLY:C   | 31:DJ:109:LEU:H    | 2.27                     | 0.42              |
| 33:DL:99:ASN:C    | 33:DL:100:ILE:HG13 | 2.44                     | 0.42              |
| 34:DM:33:LEU:H    | 34:DM:101:VAL:HB   | 1.85                     | 0.42              |
| 34:DM:38:ARG:HD3  | 34:DM:39:GLY:N     | 2.35                     | 0.42              |
| 34:DM:127:LYS:NZ  | 34:DM:129:THR:N    | 2.68                     | 0.42              |
| 35:DN:7:GLY:O     | 35:DN:8:ARG:HB2    | 2.20                     | 0.42              |
| 35:DN:34:ILE:HG22 | 35:DN:35:LYS:N     | 2.28                     | 0.42              |
| 35:DN:106:ASP:OD1 | 35:DN:106:ASP:C    | 2.63                     | 0.42              |
| 37:DP:73:PHE:CD2  | 37:DP:75:THR:HG23  | 2.55                     | 0.42              |
| 38:DQ:65:ASN:CB   | 38:DQ:75:TYR:HB2   | 2.49                     | 0.42              |
| 38:DQ:101:ASP:CG  | 38:DQ:103:VAL:HG23 | 2.44                     | 0.42              |
| 39:DR:22:LEU:CD1  | 39:DR:23:GLU:H     | 2.28                     | 0.42              |
| 39:DR:46:GLU:HB3  | 39:DR:47:VAL:H     | 1.63                     | 0.42              |
| 42:DU:24:VAL:C    | 42:DU:25:LYS:HD2   | 2.45                     | 0.42              |
| 42:DU:49:PRO:CD   | 42:DU:50:ALA:H     | 2.30                     | 0.42              |
| 44:DX:31:GLN:HE21 | 44:DX:31:GLN:CA    | 2.24                     | 0.42              |
| 49:D2:38:GLY:C    | 49:D2:39:ARG:HD2   | 2.45                     | 0.42              |
| 52:DI:63:ASP:O    | 52:DI:63:ASP:OD1   | 2.38                     | 0.42              |
| 1:AA:6:G:H4'      | 1:AA:298:A:H4'     | 2.01                     | 0.42              |
| 1:AA:109:A:N1     | 1:AA:326:G:C6      | 2.88                     | 0.42              |
| 1:AA:113:G:H21    | 1:AA:353:A:H8      | 1.66                     | 0.42              |
| 1:AA:538:G:H2'    | 1:AA:539:A:H8      | 1.85                     | 0.42              |
| 1:AA:811:C:O2'    | 1:AA:901:A:N1      | 2.47                     | 0.42              |
| 1:AA:839:C:O2'    | 1:AA:840:C:H5'     | 2.19                     | 0.42              |
| 1:AA:959:A:H2'    | 1:AA:960:U:O4'     | 2.20                     | 0.42              |
| 1:AA:960:U:O2'    | 1:AA:1223:C:H4'    | 2.20                     | 0.42              |
| 1:AA:1110:A:C5    | 1:AA:1111:A:N7     | 2.88                     | 0.42              |
| 1:AA:1473:G:O2'   | 23:BB:1702:G:H4'   | 2.20                     | 0.42              |
| 2:AC:5:HIS:CG     | 13:AN:88:MET:HB3   | 2.55                     | 0.42              |
| 2:AC:57:GLU:O     | 2:AC:63:ILE:HA     | 2.20                     | 0.42              |
| 3:AD:54:LEU:HA    | 3:AD:57:LYS:HB3    | 2.02                     | 0.42              |
| 3:AD:137:SER:HB2  | 3:AD:138:PRO:CD    | 2.45                     | 0.42              |
| 4:AE:82:HIS:CD2   | 7:AH:95:MET:HG3    | 2.55                     | 0.42              |
| 5:AF:70:VAL:HA    | 5:AF:73:GLU:HG3    | 2.02                     | 0.42              |
| 9:AJ:10:LEU:O     | 9:AJ:71:LEU:HA     | 2.19                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:AL:41:PRO:HG3   | 11:AL:46:SER:O     | 2.19                     | 0.42              |
| 12:AM:106:ARG:HA   | 12:AM:106:ARG:HD3  | 1.90                     | 0.42              |
| 13:AN:1:ALA:O      | 13:AN:5:MET:HB2    | 2.19                     | 0.42              |
| 13:AN:5:MET:C      | 13:AN:7:ALA:H      | 2.27                     | 0.42              |
| 16:AQ:9:GLY:O      | 16:AQ:58:VAL:HG22  | 2.20                     | 0.42              |
| 18:AS:47:THR:C     | 18:AS:48:ILE:HD12  | 2.45                     | 0.42              |
| 20:AB:65:LYS:HB2   | 20:AB:157:PRO:HA   | 2.02                     | 0.42              |
| 20:AB:107:ARG:HA   | 20:AB:110:ILE:HD12 | 2.01                     | 0.42              |
| 23:BB:39:G:H2'     | 23:BB:40:U:H6      | 1.84                     | 0.42              |
| 23:BB:953:G:H2'    | 23:BB:954:G:H8     | 1.85                     | 0.42              |
| 23:BB:1030:C:O2'   | 23:BB:1031:G:H5'   | 2.20                     | 0.42              |
| 23:BB:1557:C:H3'   | 23:BB:1558:C:C5'   | 2.49                     | 0.42              |
| 23:BB:1700:A:C2'   | 23:BB:1701:A:H5'   | 2.44                     | 0.42              |
| 23:BB:1783:A:H5'   | 23:BB:2608:G:H4'   | 2.02                     | 0.42              |
| 23:BB:1799:G:O2'   | 25:BC:181:ARG:HD2  | 2.19                     | 0.42              |
| 23:BB:1829:A:H3'   | 23:BB:1830:C:C6    | 2.55                     | 0.42              |
| 23:BB:1897:G:O2'   | 23:BB:1898:U:H5'   | 2.20                     | 0.42              |
| 23:BB:2047:C:O2'   | 23:BB:2823:A:N1    | 2.51                     | 0.42              |
| 23:BB:2078:C:H2'   | 23:BB:2079:U:C6    | 2.55                     | 0.42              |
| 23:BB:2245:U:O2'   | 23:BB:2436:G:OP2   | 2.37                     | 0.42              |
| 23:BB:2328:A:O2'   | 23:BB:2329:U:H5'   | 2.19                     | 0.42              |
| 23:BB:2684:U:OP1   | 37:BP:59:THR:HG22  | 2.19                     | 0.42              |
| 23:BB:2849:U:O4'   | 23:BB:2868:A:C6    | 2.73                     | 0.42              |
| 24:BV:41:GLU:C     | 24:BV:42:LEU:HD23  | 2.45                     | 0.42              |
| 25:BC:48:ILE:HG22  | 25:BC:49:THR:N     | 2.35                     | 0.42              |
| 25:BC:161:VAL:HB   | 25:BC:193:GLU:OE2  | 2.20                     | 0.42              |
| 25:BC:180:MET:HB2  | 25:BC:265:PHE:CB   | 2.49                     | 0.42              |
| 25:BC:183:VAL:O    | 25:BC:184:GLU:C    | 2.63                     | 0.42              |
| 25:BC:242:HIS:N    | 25:BC:243:PRO:HD3  | 2.34                     | 0.42              |
| 26:BD:2:ILE:HG23   | 26:BD:3:GLY:N      | 2.33                     | 0.42              |
| 26:BD:38:LYS:O     | 26:BD:42:ASN:ND2   | 2.49                     | 0.42              |
| 27:BE:152:GLU:H    | 27:BE:171:ASP:CB   | 2.33                     | 0.42              |
| 28:BF:56:LEU:HD23  | 28:BF:59:ILE:CG2   | 2.50                     | 0.42              |
| 29:BG:66:THR:O     | 29:BG:70:LEU:HB2   | 2.20                     | 0.42              |
| 29:BG:132:LEU:HD21 | 29:BG:147:LEU:CD1  | 2.49                     | 0.42              |
| 30:BH:82:SER:HB3   | 30:BH:90:LEU:HD23  | 2.02                     | 0.42              |
| 30:BH:142:VAL:HG12 | 30:BH:143:ILE:H    | 1.84                     | 0.42              |
| 32:BK:109:SER:O    | 32:BK:110:GLU:C    | 2.63                     | 0.42              |
| 33:BL:38:GLN:N     | 33:BL:41:ARG:NH1   | 2.68                     | 0.42              |
| 34:BM:3:GLN:HG2    | 34:BM:46:ILE:CB    | 2.44                     | 0.42              |
| 34:BM:75:GLU:O     | 34:BM:86:LYS:HB2   | 2.20                     | 0.42              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:BN:12:ARG:HD3   | 35:BN:20:MET:CE   | 2.50                     | 0.42              |
| 36:BO:55:GLU:HG3   | 36:BO:56:LYS:H    | 1.84                     | 0.42              |
| 37:BP:80:VAL:O     | 37:BP:80:VAL:HG22 | 2.20                     | 0.42              |
| 37:BP:91:VAL:HG12  | 37:BP:92:ARG:N    | 2.35                     | 0.42              |
| 41:BT:84:TYR:O     | 41:BT:85:VAL:O    | 2.38                     | 0.42              |
| 41:BT:89:GLU:N     | 41:BT:89:GLU:CD   | 2.77                     | 0.42              |
| 43:BW:44:PHE:N     | 43:BW:76:ARG:HB2  | 2.35                     | 0.42              |
| 47:B0:49:ARG:HG2   | 47:B0:49:ARG:O    | 2.20                     | 0.42              |
| 49:B2:34:ARG:HG3   | 49:B2:34:ARG:NH1  | 2.35                     | 0.42              |
| 50:B3:12:ARG:HG2   | 50:B3:23:HIS:CB   | 2.50                     | 0.42              |
| 52:BI:5:GLN:CG     | 52:BI:6:ALA:N     | 2.81                     | 0.42              |
| 52:BI:12:VAL:HG23  | 52:BI:41:PHE:CZ   | 2.55                     | 0.42              |
| 1:CA:123:U:H2'     | 1:CA:124:C:C6     | 2.54                     | 0.42              |
| 1:CA:280:C:N3      | 16:CQ:39:ARG:HA   | 2.35                     | 0.42              |
| 1:CA:415:A:N3      | 1:CA:415:A:O4'    | 2.53                     | 0.42              |
| 1:CA:635:A:H2'     | 1:CA:636:U:H6     | 1.85                     | 0.42              |
| 1:CA:688:G:O2'     | 1:CA:689:C:H5'    | 2.20                     | 0.42              |
| 1:CA:989:U:O2'     | 1:CA:990:C:H5'    | 2.20                     | 0.42              |
| 1:CA:1053:G:H4'    | 1:CA:1054:C:H5'   | 2.00                     | 0.42              |
| 1:CA:1381:U:O2'    | 1:CA:1382:C:H5'   | 2.20                     | 0.42              |
| 1:CA:1499:A:H1'    | 1:CA:1520:C:H5'   | 2.01                     | 0.42              |
| 2:CC:28:PHE:CZ     | 13:CN:93:PRO:HG2  | 2.55                     | 0.42              |
| 2:CC:37:LYS:HB3    | 2:CC:41:TYR:CZ    | 2.55                     | 0.42              |
| 2:CC:163:ARG:O     | 2:CC:164:THR:HG23 | 2.20                     | 0.42              |
| 4:CE:17:VAL:O      | 4:CE:17:VAL:HG22  | 2.20                     | 0.42              |
| 5:CF:29:ILE:HG23   | 5:CF:66:ALA:HB2   | 2.02                     | 0.42              |
| 6:CG:55:LYS:CG     | 6:CG:56:SER:H     | 2.30                     | 0.42              |
| 6:CG:56:SER:HB3    | 6:CG:59:GLU:CB    | 2.50                     | 0.42              |
| 9:CJ:9:ARG:HG3     | 9:CJ:99:GLN:HB2   | 2.01                     | 0.42              |
| 13:CN:26:LEU:HA    | 13:CN:29:ILE:CD1  | 2.44                     | 0.42              |
| 13:CN:30:ILE:H     | 13:CN:44:VAL:HG21 | 1.85                     | 0.42              |
| 14:CO:69:LEU:HD21  | 14:CO:76:ARG:HD2  | 2.02                     | 0.42              |
| 15:CP:1:MET:HA     | 15:CP:1:MET:HE3   | 2.00                     | 0.42              |
| 15:CP:12:LYS:HD2   | 15:CP:13:LYS:HG3  | 2.02                     | 0.42              |
| 15:CP:67:ILE:HG13  | 15:CP:71:VAL:CG1  | 2.40                     | 0.42              |
| 18:CS:30:LEU:HB2   | 18:CS:48:ILE:HG12 | 2.01                     | 0.42              |
| 18:CS:46:LEU:HB3   | 18:CS:47:THR:H    | 1.73                     | 0.42              |
| 19:CT:47:GLN:HG2   | 19:CT:82:ILE:HD12 | 2.01                     | 0.42              |
| 20:CB:27:LYS:CB    | 20:CB:28:PRO:HD3  | 2.46                     | 0.42              |
| 20:CB:209:VAL:HG23 | 20:CB:210:THR:H   | 1.85                     | 0.42              |
| 23:DB:161:A:H3'    | 23:DB:162:U:C5'   | 2.38                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DB:162:U:O2'    | 23:DB:163:C:C5'   | 2.60                     | 0.42              |
| 23:DB:211:C:O2'    | 23:DB:212:G:H5'   | 2.20                     | 0.42              |
| 23:DB:409:G:H2'    | 23:DB:410:G:H8    | 1.85                     | 0.42              |
| 23:DB:459:U:O2'    | 23:DB:460:A:H5'   | 2.20                     | 0.42              |
| 23:DB:647:G:H2'    | 23:DB:648:G:H8    | 1.85                     | 0.42              |
| 23:DB:1099:G:C8    | 52:DI:3:LYS:O     | 2.73                     | 0.42              |
| 23:DB:1399:C:O2'   | 23:DB:1400:U:H5'  | 2.20                     | 0.42              |
| 23:DB:1665:A:H1'   | 32:DK:67:LYS:HE2  | 2.02                     | 0.42              |
| 23:DB:1674:G:N2    | 23:DB:1677:A:N1   | 2.67                     | 0.42              |
| 23:DB:1713:A:N6    | 23:DB:1745:A:H61  | 2.18                     | 0.42              |
| 23:DB:1791:A:C2    | 23:DB:1829:A:O4'  | 2.73                     | 0.42              |
| 23:DB:2266:A:O4'   | 23:DB:2272:U:O4   | 2.37                     | 0.42              |
| 23:DB:2347:C:OP1   | 23:DB:2347:C:H4'  | 2.19                     | 0.42              |
| 23:DB:2527:C:H4'   | 51:D4:34:LYS:O    | 2.20                     | 0.42              |
| 25:DC:91:ALA:O     | 25:DC:102:TYR:HD2 | 2.03                     | 0.42              |
| 25:DC:103:ILE:CG2  | 25:DC:104:LEU:H   | 2.33                     | 0.42              |
| 25:DC:161:VAL:HG12 | 25:DC:161:VAL:O   | 2.19                     | 0.42              |
| 25:DC:257:ARG:HA   | 25:DC:261:ARG:CZ  | 2.49                     | 0.42              |
| 26:DD:32:ASN:O     | 26:DD:34:VAL:HG13 | 2.20                     | 0.42              |
| 26:DD:34:VAL:HG11  | 26:DD:50:VAL:CG2  | 2.50                     | 0.42              |
| 26:DD:178:VAL:C    | 26:DD:179:ARG:HG2 | 2.45                     | 0.42              |
| 27:DE:164:LEU:HD13 | 27:DE:164:LEU:C   | 2.45                     | 0.42              |
| 27:DE:169:VAL:O    | 27:DE:170:ARG:HB2 | 2.19                     | 0.42              |
| 28:DF:163:GLU:HA   | 28:DF:166:ARG:CG  | 2.50                     | 0.42              |
| 29:DG:29:ASN:OD1   | 29:DG:81:GLY:HA2  | 2.19                     | 0.42              |
| 29:DG:155:PRO:O    | 29:DG:171:LYS:HG3 | 2.19                     | 0.42              |
| 30:DH:35:LYS:O     | 30:DH:35:LYS:HG3  | 2.20                     | 0.42              |
| 30:DH:101:ASP:O    | 30:DH:104:THR:HB  | 2.19                     | 0.42              |
| 30:DH:131:SER:HB2  | 30:DH:141:LYS:HG3 | 2.02                     | 0.42              |
| 30:DH:144:VAL:HG12 | 30:DH:145:ASN:N   | 2.34                     | 0.42              |
| 31:DJ:44:TYR:CE2   | 31:DJ:50:THR:HB   | 2.54                     | 0.42              |
| 31:DJ:96:ARG:HG2   | 31:DJ:99:ARG:HB2  | 2.01                     | 0.42              |
| 34:DM:1:MET:HA     | 34:DM:1:MET:HE2   | 2.02                     | 0.42              |
| 34:DM:16:ARG:HH11  | 34:DM:16:ARG:CG   | 2.33                     | 0.42              |
| 34:DM:114:ARG:C    | 34:DM:116:ALA:N   | 2.76                     | 0.42              |
| 35:DN:12:ARG:HB3   | 35:DN:13:ASN:H    | 1.77                     | 0.42              |
| 37:DP:18:SER:HA    | 37:DP:87:ARG:HH22 | 1.85                     | 0.42              |
| 38:DQ:74:SER:O     | 38:DQ:75:TYR:C    | 2.63                     | 0.42              |
| 38:DQ:92:LYS:O     | 38:DQ:94:LEU:N    | 2.53                     | 0.42              |
| 41:DT:53:VAL:HB    | 41:DT:87:LEU:HD21 | 2.02                     | 0.42              |
| 42:DU:40:LEU:O     | 42:DU:58:VAL:HA   | 2.19                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:DW:75:ASN:O    | 43:DW:77:LYS:N    | 2.52                     | 0.42              |
| 44:DX:55:THR:O    | 44:DX:57:LEU:N    | 2.40                     | 0.42              |
| 46:DZ:59:ARG:O    | 46:DZ:60:PHE:HB3  | 2.20                     | 0.42              |
| 50:D3:46:LYS:HD2  | 50:D3:47:ALA:N    | 2.35                     | 0.42              |
| 52:DI:117:THR:O   | 52:DI:118:GLY:C   | 2.61                     | 0.42              |
| 1:AA:207:C:O2'    | 1:AA:208:U:H5'    | 2.20                     | 0.41              |
| 1:AA:208:U:C2'    | 1:AA:209:U:H5''   | 2.50                     | 0.41              |
| 1:AA:412:A:H1'    | 1:AA:413:G:C8     | 2.46                     | 0.41              |
| 1:AA:821:G:H2'    | 1:AA:822:U:C6     | 2.55                     | 0.41              |
| 1:AA:952:U:O2'    | 1:AA:953:G:H5'    | 2.20                     | 0.41              |
| 1:AA:1052:U:H5'   | 1:AA:1053:G:OP2   | 2.20                     | 0.41              |
| 2:AC:24:ASN:O     | 2:AC:26:LYS:N     | 2.54                     | 0.41              |
| 2:AC:172:VAL:HG11 | 2:AC:200:TRP:HB3  | 2.02                     | 0.41              |
| 4:AE:82:HIS:HE1   | 4:AE:147:ASN:H    | 1.67                     | 0.41              |
| 4:AE:137:ARG:HG2  | 4:AE:137:ARG:H    | 1.75                     | 0.41              |
| 8:AI:15:ALA:O     | 8:AI:66:VAL:HA    | 2.20                     | 0.41              |
| 9:AJ:93:ALA:HB1   | 9:AJ:96:VAL:HG23  | 2.02                     | 0.41              |
| 10:AK:22:ILE:HG23 | 10:AK:31:VAL:HG22 | 2.02                     | 0.41              |
| 10:AK:105:ARG:HB3 | 10:AK:106:ILE:H   | 1.65                     | 0.41              |
| 10:AK:121:ARG:NH1 | 10:AK:121:ARG:HG3 | 2.34                     | 0.41              |
| 13:AN:19:TYR:HE2  | 13:AN:23:ARG:NH1  | 2.17                     | 0.41              |
| 13:AN:20:PHE:HA   | 13:AN:24:ALA:H    | 1.85                     | 0.41              |
| 14:AO:52:ARG:O    | 14:AO:55:LEU:HB3  | 2.20                     | 0.41              |
| 15:AP:8:ARG:NE    | 15:AP:15:PRO:HB3  | 2.34                     | 0.41              |
| 15:AP:51:ARG:O    | 15:AP:52:LEU:HD13 | 2.19                     | 0.41              |
| 15:AP:68:SER:HB3  | 15:AP:71:VAL:CG1  | 2.47                     | 0.41              |
| 18:AS:44:ILE:HA   | 18:AS:61:VAL:HB   | 2.01                     | 0.41              |
| 22:BA:50:A:OP1    | 36:BO:68:LYS:HG3  | 2.19                     | 0.41              |
| 22:BA:75:G:H1'    | 24:BV:29:ILE:HG21 | 2.01                     | 0.41              |
| 23:BB:58:G:H2'    | 23:BB:59:U:C6     | 2.55                     | 0.41              |
| 23:BB:136:G:H8    | 23:BB:136:G:P     | 2.43                     | 0.41              |
| 23:BB:161:A:H8    | 23:BB:161:A:O5'   | 2.02                     | 0.41              |
| 23:BB:354:A:H2'   | 23:BB:355:U:O4'   | 2.20                     | 0.41              |
| 23:BB:433:C:H2'   | 23:BB:434:U:H6    | 1.84                     | 0.41              |
| 23:BB:482:A:H5''  | 42:BU:43:LYS:CE   | 2.33                     | 0.41              |
| 23:BB:508:A:H2'   | 23:BB:509:C:C5'   | 2.45                     | 0.41              |
| 23:BB:522:A:H2'   | 23:BB:523:C:H6    | 1.85                     | 0.41              |
| 23:BB:636:G:N1    | 33:BL:76:GLU:OE2  | 2.53                     | 0.41              |
| 23:BB:647:G:H2'   | 23:BB:648:G:H8    | 1.85                     | 0.41              |
| 23:BB:908:C:O2'   | 23:BB:909:A:H5'   | 2.20                     | 0.41              |
| 23:BB:1082:U:H2'  | 23:BB:1083:U:O4'  | 2.20                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BB:1132:U:H5'  | 31:BJ:85:LYS:HZ3  | 1.83                     | 0.41              |
| 23:BB:1236:G:O2'  | 23:BB:1237:A:O4'  | 2.36                     | 0.41              |
| 23:BB:1268:A:H2'  | 23:BB:1269:A:C8   | 2.55                     | 0.41              |
| 23:BB:1289:C:C2   | 23:BB:1290:C:C5   | 3.07                     | 0.41              |
| 23:BB:1294:U:C4   | 23:BB:1295:C:C5   | 3.07                     | 0.41              |
| 23:BB:1372:U:H2'  | 23:BB:1373:A:H8   | 1.86                     | 0.41              |
| 23:BB:1529:G:H2'  | 23:BB:1530:G:H8   | 1.85                     | 0.41              |
| 23:BB:1678:A:C2'  | 23:BB:1679:A:H5'  | 2.50                     | 0.41              |
| 23:BB:2026:U:C2   | 23:BB:2027:G:C8   | 3.07                     | 0.41              |
| 23:BB:2046:G:H5'  | 47:B0:15:ARG:HG3  | 2.01                     | 0.41              |
| 23:BB:2047:C:OP1  | 47:B0:15:ARG:HD2  | 2.20                     | 0.41              |
| 23:BB:2270:A:O5'  | 43:BW:18:LYS:HB3  | 2.19                     | 0.41              |
| 23:BB:2308:G:H5'  | 23:BB:2309:A:C5'  | 2.49                     | 0.41              |
| 23:BB:2322:A:C6   | 23:BB:2333:A:N6   | 2.88                     | 0.41              |
| 23:BB:2324:U:O2'  | 23:BB:2385:C:H5   | 2.02                     | 0.41              |
| 23:BB:2708:G:O2'  | 23:BB:2709:G:H5'  | 2.20                     | 0.41              |
| 25:BC:51:ARG:O    | 25:BC:51:ARG:NE   | 2.52                     | 0.41              |
| 26:BD:100:LEU:O   | 26:BD:100:LEU:HG  | 2.20                     | 0.41              |
| 27:BE:84:THR:CG2  | 27:BE:85:PHE:H    | 2.26                     | 0.41              |
| 30:BH:89:LYS:HE2  | 30:BH:90:LEU:N    | 2.35                     | 0.41              |
| 30:BH:98:ASP:O    | 30:BH:102:ALA:HB2 | 2.20                     | 0.41              |
| 32:BK:2:ILE:CD1   | 32:BK:8:LEU:HD21  | 2.50                     | 0.41              |
| 32:BK:87:LEU:O    | 32:BK:89:ASN:N    | 2.53                     | 0.41              |
| 34:BM:10:ARG:HB3  | 34:BM:11:LYS:HE3  | 2.02                     | 0.41              |
| 34:BM:84:LYS:H    | 34:BM:84:LYS:HZ3  | 1.66                     | 0.41              |
| 35:BN:65:LEU:HD12 | 35:BN:68:ALA:HB3  | 2.02                     | 0.41              |
| 35:BN:73:ASN:C    | 35:BN:76:VAL:HG13 | 2.45                     | 0.41              |
| 37:BP:52:ARG:HB3  | 37:BP:60:VAL:HG21 | 2.00                     | 0.41              |
| 38:BQ:65:ASN:HB2  | 38:BQ:75:TYR:CB   | 2.45                     | 0.41              |
| 38:BQ:94:LEU:H    | 38:BQ:94:LEU:CD1  | 2.27                     | 0.41              |
| 42:BU:92:VAL:HG22 | 42:BU:92:VAL:O    | 2.20                     | 0.41              |
| 43:BW:40:ARG:NH1  | 43:BW:68:PHE:HD1  | 2.17                     | 0.41              |
| 45:BY:28:LEU:HD12 | 45:BY:28:LEU:N    | 2.35                     | 0.41              |
| 47:B0:4:GLN:HE21  | 47:B0:4:GLN:HB3   | 1.65                     | 0.41              |
| 47:B0:15:ARG:NH1  | 47:B0:15:ARG:HG2  | 2.35                     | 0.41              |
| 48:B1:49:LYS:HD2  | 48:B1:49:LYS:H    | 1.85                     | 0.41              |
| 50:B3:24:LYS:HE2  | 50:B3:29:ARG:HH22 | 1.85                     | 0.41              |
| 50:B3:27:ASN:CG   | 50:B3:28:LEU:N    | 2.77                     | 0.41              |
| 1:CA:73:C:H2'     | 1:CA:74:A:H8      | 1.85                     | 0.41              |
| 1:CA:154:U:O2'    | 1:CA:155:A:H5'    | 2.20                     | 0.41              |
| 1:CA:262:A:H5''   | 19:CT:70:LYS:HD2  | 2.02                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:309:A:O2'    | 1:CA:607:A:N1      | 2.52                     | 0.41              |
| 1:CA:928:G:H2'    | 1:CA:929:G:H8      | 1.85                     | 0.41              |
| 1:CA:951:G:O2'    | 1:CA:952:U:H5'     | 2.19                     | 0.41              |
| 1:CA:975:A:O2'    | 1:CA:976:G:P       | 2.77                     | 0.41              |
| 1:CA:1279:G:N1    | 9:CJ:45:ARG:NH1    | 2.68                     | 0.41              |
| 1:CA:1292:G:O2'   | 1:CA:1293:C:H5'    | 2.20                     | 0.41              |
| 1:CA:1307:U:H2'   | 1:CA:1308:U:O4'    | 2.19                     | 0.41              |
| 2:CC:53:ARG:O     | 2:CC:67:ILE:HD12   | 2.20                     | 0.41              |
| 2:CC:63:ILE:O     | 2:CC:63:ILE:HG23   | 2.19                     | 0.41              |
| 3:CD:24:VAL:HG23  | 3:CD:25:ARG:N      | 2.35                     | 0.41              |
| 3:CD:97:LEU:HB2   | 3:CD:134:TYR:HB3   | 2.02                     | 0.41              |
| 3:CD:169:TRP:HB2  | 3:CD:183:ARG:O     | 2.20                     | 0.41              |
| 5:CF:11:HIS:NE2   | 5:CF:13:ASP:HB3    | 2.34                     | 0.41              |
| 5:CF:85:ILE:CG2   | 5:CF:86:ARG:H      | 2.32                     | 0.41              |
| 8:CI:105:ARG:O    | 8:CI:107:ALA:N     | 2.53                     | 0.41              |
| 9:CJ:65:TYR:CE1   | 13:CN:84:ARG:HA    | 2.54                     | 0.41              |
| 10:CK:94:SER:HA   | 10:CK:97:ARG:CG    | 2.50                     | 0.41              |
| 13:CN:51:PRO:HG2  | 13:CN:52:ARG:N     | 2.30                     | 0.41              |
| 14:CO:44:GLU:O    | 14:CO:45:HIS:C     | 2.63                     | 0.41              |
| 16:CQ:45:VAL:HA   | 16:CQ:72:TRP:O     | 2.20                     | 0.41              |
| 18:CS:10:ILE:HG23 | 18:CS:40:PHE:HE2   | 1.85                     | 0.41              |
| 20:CB:181:PRO:HA  | 20:CB:196:ASP:OD2  | 2.19                     | 0.41              |
| 23:DB:35:G:H2'    | 23:DB:36:G:O4'     | 2.20                     | 0.41              |
| 23:DB:327:G:H2'   | 23:DB:328:U:O4'    | 2.20                     | 0.41              |
| 23:DB:397:U:OP1   | 46:DZ:48:GLN:HG3   | 2.20                     | 0.41              |
| 23:DB:608:A:H2'   | 23:DB:609:A:H8     | 1.81                     | 0.41              |
| 23:DB:775:G:C5    | 23:DB:794:A:C8     | 3.08                     | 0.41              |
| 23:DB:1112:G:H5'  | 29:DG:1:SER:HA     | 2.01                     | 0.41              |
| 23:DB:1221:C:O2'  | 23:DB:1222:U:H5'   | 2.20                     | 0.41              |
| 23:DB:1274:A:N1   | 23:DB:1644:C:O2'   | 2.50                     | 0.41              |
| 23:DB:1373:A:OP1  | 23:DB:2213:U:C4    | 2.73                     | 0.41              |
| 23:DB:1421:G:C2   | 23:DB:1422:G:C8    | 3.08                     | 0.41              |
| 23:DB:1529:G:H2'  | 23:DB:1530:G:H8    | 1.85                     | 0.41              |
| 23:DB:1541:C:H2'  | 23:DB:1542:U:H6    | 1.85                     | 0.41              |
| 23:DB:1788:C:O2'  | 23:DB:1789:A:H5'   | 2.20                     | 0.41              |
| 23:DB:1812:U:H2'  | 23:DB:1813:G:C8    | 2.53                     | 0.41              |
| 23:DB:2091:C:H1'  | 46:DZ:32:LEU:HG    | 2.02                     | 0.41              |
| 23:DB:2708:G:O2'  | 23:DB:2709:G:H5'   | 2.20                     | 0.41              |
| 25:DC:22:GLU:HA   | 25:DC:202:ARG:CZ   | 2.50                     | 0.41              |
| 28:DF:132:ARG:HG3 | 28:DF:132:ARG:HH11 | 1.85                     | 0.41              |
| 29:DG:62:ALA:C    | 29:DG:64:ALA:N     | 2.78                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:DH:3:VAL:CG2    | 30:DH:37:VAL:HG21  | 2.49                     | 0.41              |
| 31:DJ:41:LYS:O     | 38:DQ:63:ARG:NH2   | 2.53                     | 0.41              |
| 32:DK:63:VAL:CG2   | 32:DK:115:ILE:HD11 | 2.50                     | 0.41              |
| 34:DM:81:ARG:O     | 34:DM:82:MET:C     | 2.63                     | 0.41              |
| 34:DM:112:LEU:O    | 34:DM:113:ALA:C    | 2.63                     | 0.41              |
| 35:DN:54:LEU:HD23  | 35:DN:54:LEU:C     | 2.45                     | 0.41              |
| 36:DO:10:ARG:HG3   | 36:DO:96:GLY:N     | 2.35                     | 0.41              |
| 39:DR:32:THR:HA    | 39:DR:35:PHE:CE2   | 2.55                     | 0.41              |
| 40:DS:8:ARG:HA     | 40:DS:102:HIS:ND1  | 2.35                     | 0.41              |
| 40:DS:42:LYS:HD3   | 40:DS:42:LYS:C     | 2.46                     | 0.41              |
| 42:DU:36:GLU:O     | 42:DU:37:GLY:C     | 2.62                     | 0.41              |
| 43:DW:7:GLY:C      | 43:DW:9:THR:H      | 2.26                     | 0.41              |
| 47:D0:12:ARG:HG3   | 47:D0:13:GLY:N     | 2.35                     | 0.41              |
| 48:D1:8:ILE:HB     | 48:D1:27:ARG:NH1   | 2.35                     | 0.41              |
| 1:AA:372:C:C1'     | 1:AA:373:A:OP2     | 2.66                     | 0.41              |
| 1:AA:598:U:C2      | 1:AA:599:C:C5      | 3.09                     | 0.41              |
| 1:AA:981:U:P       | 13:AN:12:ARG:HH12  | 2.42                     | 0.41              |
| 1:AA:1414:U:H2'    | 1:AA:1415:G:C8     | 2.55                     | 0.41              |
| 2:AC:82:ASP:O      | 2:AC:86:LEU:HG     | 2.19                     | 0.41              |
| 2:AC:131:ARG:CZ    | 2:AC:131:ARG:HB3   | 2.50                     | 0.41              |
| 2:AC:186:SER:HB3   | 2:AC:197:VAL:CG1   | 2.50                     | 0.41              |
| 3:AD:43:ARG:HB3    | 3:AD:44:LYS:H      | 1.48                     | 0.41              |
| 3:AD:132:ALA:C     | 3:AD:134:TYR:H     | 2.28                     | 0.41              |
| 4:AE:61:LYS:O      | 4:AE:65:LYS:HG2    | 2.20                     | 0.41              |
| 4:AE:63:MET:O      | 4:AE:66:ALA:HB3    | 2.20                     | 0.41              |
| 6:AG:96:ASN:O      | 6:AG:100:MET:HG3   | 2.20                     | 0.41              |
| 6:AG:138:GLU:C     | 6:AG:140:VAL:N     | 2.77                     | 0.41              |
| 8:AI:56:MET:HE2    | 8:AI:56:MET:HB2    | 1.76                     | 0.41              |
| 10:AK:41:LEU:C     | 10:AK:73:VAL:HG13  | 2.45                     | 0.41              |
| 14:AO:80:LEU:O     | 14:AO:84:LEU:HD13  | 2.20                     | 0.41              |
| 17:AR:70:THR:OG1   | 17:AR:71:ASP:N     | 2.52                     | 0.41              |
| 20:AB:14:HIS:NE2   | 20:AB:49:PHE:HZ    | 2.17                     | 0.41              |
| 20:AB:185:ILE:HD12 | 20:AB:185:ILE:O    | 2.20                     | 0.41              |
| 22:BA:92:C:H2'     | 22:BA:93:C:H6      | 1.84                     | 0.41              |
| 23:BB:30:G:H2'     | 23:BB:31:C:H6      | 1.85                     | 0.41              |
| 23:BB:1010:A:O2'   | 23:BB:1152:C:H1'   | 2.20                     | 0.41              |
| 23:BB:1119:U:H2'   | 23:BB:1120:G:H8    | 1.85                     | 0.41              |
| 23:BB:1215:G:O2'   | 23:BB:1216:G:H5'   | 2.20                     | 0.41              |
| 23:BB:1998:A:H2'   | 23:BB:1999:C:C6    | 2.55                     | 0.41              |
| 23:BB:2149:U:OP1   | 23:BB:2149:U:H4'   | 2.20                     | 0.41              |
| 23:BB:2185:U:O5'   | 23:BB:2185:U:H6    | 2.02                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:BB:2462:C:H2'   | 23:BB:2463:C:H6   | 1.84                     | 0.41              |
| 23:BB:2513:A:H2'   | 23:BB:2514:U:C6   | 2.55                     | 0.41              |
| 23:BB:2526:G:N2    | 51:B4:1:MET:HB3   | 2.35                     | 0.41              |
| 23:BB:2572:A:C2    | 26:BD:150:GLN:NE2 | 2.88                     | 0.41              |
| 23:BB:2673:G:H2'   | 23:BB:2674:G:H8   | 1.85                     | 0.41              |
| 23:BB:2723:C:H5''  | 35:BN:3:HIS:HB2   | 2.03                     | 0.41              |
| 23:BB:2768:U:H2'   | 23:BB:2769:U:O4'  | 2.20                     | 0.41              |
| 23:BB:2849:U:N3    | 23:BB:2867:G:H1'  | 2.35                     | 0.41              |
| 24:BV:6:ALA:HB3    | 24:BV:65:VAL:CG1  | 2.50                     | 0.41              |
| 25:BC:27:LYS:N     | 25:BC:28:PRO:CD   | 2.83                     | 0.41              |
| 25:BC:78:GLU:HB3   | 25:BC:92:LEU:HD23 | 2.02                     | 0.41              |
| 25:BC:163:ILE:CG2  | 25:BC:164:VAL:H   | 2.17                     | 0.41              |
| 25:BC:251:THR:HG22 | 25:BC:252:LYS:N   | 2.34                     | 0.41              |
| 26:BD:33:ARG:O     | 26:BD:34:VAL:HB   | 2.19                     | 0.41              |
| 31:BJ:66:GLY:C     | 31:BJ:68:LYS:H    | 2.26                     | 0.41              |
| 33:BL:47:ARG:O     | 33:BL:47:ARG:HG3  | 2.20                     | 0.41              |
| 33:BL:74:THR:O     | 33:BL:75:ALA:C    | 2.63                     | 0.41              |
| 36:BO:39:VAL:HB    | 36:BO:83:LEU:CD1  | 2.49                     | 0.41              |
| 36:BO:49:VAL:CG2   | 36:BO:50:ALA:H    | 2.19                     | 0.41              |
| 40:BS:8:ARG:NH1    | 40:BS:102:HIS:NE2 | 2.67                     | 0.41              |
| 41:BT:16:VAL:O     | 41:BT:16:VAL:HG13 | 2.20                     | 0.41              |
| 42:BU:35:VAL:CG1   | 42:BU:36:GLU:H    | 2.15                     | 0.41              |
| 42:BU:71:ILE:HG23  | 42:BU:72:PHE:N    | 2.35                     | 0.41              |
| 43:BW:35:ILE:HG12  | 43:BW:70:VAL:CG2  | 2.47                     | 0.41              |
| 46:BZ:54:GLY:C     | 46:BZ:56:ARG:H    | 2.29                     | 0.41              |
| 51:B4:24:ARG:HG2   | 51:B4:26:ILE:HG12 | 2.02                     | 0.41              |
| 1:CA:102:G:N3      | 1:CA:151:A:H2     | 2.18                     | 0.41              |
| 1:CA:155:A:H2'     | 1:CA:156:C:O4'    | 2.19                     | 0.41              |
| 1:CA:208:U:H2'     | 1:CA:210:C:C5     | 2.55                     | 0.41              |
| 1:CA:392:C:H2'     | 1:CA:393:A:C8     | 2.54                     | 0.41              |
| 1:CA:407:U:H3'     | 1:CA:408:A:H8     | 1.85                     | 0.41              |
| 1:CA:562:U:H1'     | 11:CL:11:ARG:HB3  | 2.02                     | 0.41              |
| 1:CA:839:C:O2'     | 1:CA:840:C:H5'    | 2.19                     | 0.41              |
| 1:CA:949:A:H2'     | 1:CA:950:U:O4'    | 2.21                     | 0.41              |
| 1:CA:1148:U:H2'    | 1:CA:1149:C:O4'   | 2.19                     | 0.41              |
| 1:CA:1320:C:H41    | 18:CS:36:ARG:CG   | 2.32                     | 0.41              |
| 1:CA:1483:A:H2'    | 1:CA:1484:C:O4'   | 2.20                     | 0.41              |
| 1:CA:1493:A:H2'    | 1:CA:1494:G:OP2   | 2.20                     | 0.41              |
| 3:CD:151:GLN:HE21  | 3:CD:153:ARG:HB3  | 1.85                     | 0.41              |
| 3:CD:171:GLU:O     | 3:CD:180:THR:HB   | 2.21                     | 0.41              |
| 7:CH:28:SER:HB3    | 7:CH:58:LEU:HB2   | 2.01                     | 0.41              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:CI:80:HIS:HE1   | 8:CI:103:VAL:O     | 2.03                     | 0.41              |
| 10:CK:22:ILE:HD13 | 10:CK:95:THR:CG2   | 2.49                     | 0.41              |
| 10:CK:70:ALA:CA   | 10:CK:74:LYS:HB2   | 2.50                     | 0.41              |
| 10:CK:126:ARG:HG2 | 10:CK:126:ARG:NH1  | 2.35                     | 0.41              |
| 11:CL:113:ARG:O   | 11:CL:114:SER:C    | 2.61                     | 0.41              |
| 12:CM:18:LEU:HD23 | 12:CM:18:LEU:O     | 2.20                     | 0.41              |
| 13:CN:21:ALA:O    | 13:CN:24:ALA:HB3   | 2.20                     | 0.41              |
| 13:CN:65:GLN:HB3  | 13:CN:82:LYS:HG2   | 2.01                     | 0.41              |
| 13:CN:82:LYS:HE2  | 13:CN:82:LYS:HA    | 2.01                     | 0.41              |
| 22:DA:30:C:H2'    | 22:DA:31:C:C5'     | 2.41                     | 0.41              |
| 22:DA:112:G:H2'   | 22:DA:113:C:C6     | 2.54                     | 0.41              |
| 23:DB:212:G:H2'   | 23:DB:213:A:C8     | 2.55                     | 0.41              |
| 23:DB:340:A:H2'   | 23:DB:341:C:C5'    | 2.50                     | 0.41              |
| 23:DB:910:A:N7    | 34:DM:16:ARG:HB3   | 2.35                     | 0.41              |
| 23:DB:963:U:H2'   | 23:DB:964:C:H6     | 1.84                     | 0.41              |
| 23:DB:1987:A:H2'  | 23:DB:1988:G:C8    | 2.54                     | 0.41              |
| 23:DB:2016:U:H2'  | 23:DB:2017:U:C6    | 2.56                     | 0.41              |
| 23:DB:2720:U:H2'  | 23:DB:2721:A:C8    | 2.55                     | 0.41              |
| 23:DB:2768:U:H2'  | 23:DB:2769:U:O4'   | 2.20                     | 0.41              |
| 23:DB:2874:C:H2'  | 23:DB:2875:C:H6    | 1.84                     | 0.41              |
| 23:DB:2886:A:C4   | 47:D0:27:LEU:HG    | 2.56                     | 0.41              |
| 25:DC:27:LYS:HD2  | 25:DC:27:LYS:N     | 2.35                     | 0.41              |
| 25:DC:42:ARG:CZ   | 25:DC:44:ASN:HB2   | 2.50                     | 0.41              |
| 26:DD:106:LYS:HG3 | 26:DD:208:LYS:CE   | 2.51                     | 0.41              |
| 28:DF:9:ASP:O     | 28:DF:10:GLU:CB    | 2.68                     | 0.41              |
| 28:DF:36:ASN:HD22 | 28:DF:87:LYS:H     | 1.68                     | 0.41              |
| 28:DF:38:GLY:N    | 28:DF:86:CYS:SG    | 2.93                     | 0.41              |
| 28:DF:174:PHE:N   | 28:DF:175:PRO:CD   | 2.83                     | 0.41              |
| 29:DG:96:ALA:HA   | 29:DG:124:CYS:SG   | 2.60                     | 0.41              |
| 31:DJ:64:VAL:HG21 | 31:DJ:69:ARG:HG2   | 2.02                     | 0.41              |
| 31:DJ:80:HIS:ND1  | 31:DJ:80:HIS:N     | 2.68                     | 0.41              |
| 31:DJ:124:VAL:CG2 | 31:DJ:125:TYR:N    | 2.76                     | 0.41              |
| 32:DK:17:ARG:HB2  | 32:DK:45:GLU:HB3   | 2.02                     | 0.41              |
| 33:DL:79:LEU:N    | 33:DL:113:ALA:HB3  | 2.35                     | 0.41              |
| 33:DL:100:ILE:O   | 33:DL:101:ILE:HD13 | 2.19                     | 0.41              |
| 33:DL:116:VAL:O   | 33:DL:116:VAL:HG23 | 2.20                     | 0.41              |
| 34:DM:15:GLY:O    | 34:DM:16:ARG:O     | 2.38                     | 0.41              |
| 37:DP:40:GLN:O    | 37:DP:41:ALA:O     | 2.38                     | 0.41              |
| 39:DR:6:GLN:CB    | 39:DR:41:ILE:HD13  | 2.49                     | 0.41              |
| 40:DS:7:HIS:ND1   | 40:DS:7:HIS:O      | 2.52                     | 0.41              |
| 42:DU:71:ILE:CD1  | 42:DU:72:PHE:N     | 2.80                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 46:DZ:31:ASP:C     | 46:DZ:32:LEU:HD22 | 2.45                     | 0.41              |
| 48:D1:24:LYS:HB2   | 48:D1:24:LYS:NZ   | 2.31                     | 0.41              |
| 1:AA:112:G:O2'     | 1:AA:113:G:H5'    | 2.19                     | 0.41              |
| 1:AA:243:A:C1'     | 1:AA:244:U:OP2    | 2.68                     | 0.41              |
| 1:AA:254:G:H4'     | 16:AQ:19:SER:OG   | 2.20                     | 0.41              |
| 1:AA:546:A:H4'     | 1:AA:548:G:O3'    | 2.21                     | 0.41              |
| 1:AA:599:C:H2'     | 1:AA:600:A:H8     | 1.85                     | 0.41              |
| 1:AA:728:A:H2'     | 1:AA:729:A:C8     | 2.56                     | 0.41              |
| 1:AA:814:A:C5'     | 1:AA:1511:G:H4'   | 2.45                     | 0.41              |
| 1:AA:969:A:H2'     | 1:AA:970:C:O2     | 2.21                     | 0.41              |
| 1:AA:1281:C:H3'    | 1:AA:1282:C:H6    | 1.85                     | 0.41              |
| 2:AC:135:ARG:C     | 2:AC:137:VAL:N    | 2.78                     | 0.41              |
| 3:AD:12:ARG:HG3    | 3:AD:33:ILE:HA    | 2.01                     | 0.41              |
| 5:AF:42:TRP:CZ2    | 5:AF:61:LEU:HD23  | 2.55                     | 0.41              |
| 6:AG:8:GLN:HG2     | 6:AG:9:ARG:N      | 2.35                     | 0.41              |
| 6:AG:30:MET:HA     | 6:AG:38:ALA:CB    | 2.51                     | 0.41              |
| 6:AG:49:LEU:HB3    | 6:AG:57:GLU:OE2   | 2.20                     | 0.41              |
| 7:AH:45:ILE:C      | 7:AH:63:LYS:HZ1   | 2.28                     | 0.41              |
| 7:AH:113:ARG:NH2   | 7:AH:114:ALA:HA   | 2.21                     | 0.41              |
| 8:AI:20:ILE:HD13   | 8:AI:85:ALA:CB    | 2.50                     | 0.41              |
| 8:AI:56:MET:O      | 8:AI:58:GLU:N     | 2.53                     | 0.41              |
| 9:AJ:96:VAL:O      | 9:AJ:98:VAL:HG13  | 2.19                     | 0.41              |
| 11:AL:21:PRO:HD2   | 11:AL:94:TYR:OH   | 2.20                     | 0.41              |
| 12:AM:14:ALA:HB1   | 12:AM:33:LEU:HD11 | 2.02                     | 0.41              |
| 12:AM:56:ARG:C     | 12:AM:59:VAL:HG12 | 2.45                     | 0.41              |
| 16:AQ:29:LYS:HA    | 16:AQ:35:LYS:C    | 2.45                     | 0.41              |
| 17:AR:52:ARG:HH11  | 17:AR:52:ARG:CB   | 2.21                     | 0.41              |
| 18:AS:78:THR:HG22  | 18:AS:79:TYR:N    | 2.35                     | 0.41              |
| 20:AB:67:LEU:HD21  | 20:AB:157:PRO:CB  | 2.50                     | 0.41              |
| 20:AB:107:ARG:HA   | 20:AB:110:ILE:CD1 | 2.50                     | 0.41              |
| 20:AB:185:ILE:HG22 | 20:AB:199:ILE:HB  | 2.02                     | 0.41              |
| 21:AU:16:ARG:C     | 21:AU:18:PHE:N    | 2.78                     | 0.41              |
| 23:BB:79:C:H2'     | 23:BB:80:G:H8     | 1.85                     | 0.41              |
| 23:BB:107:G:H2'    | 23:BB:108:G:H8    | 1.84                     | 0.41              |
| 23:BB:118:A:H5'    | 23:BB:119:A:C8    | 2.41                     | 0.41              |
| 23:BB:277:G:HO2'   | 23:BB:361:G:H1    | 1.68                     | 0.41              |
| 23:BB:328:U:C4'    | 42:BU:65:GLN:HG3  | 2.44                     | 0.41              |
| 23:BB:410:G:C2     | 23:BB:2407:A:C5   | 3.08                     | 0.41              |
| 23:BB:583:G:H2'    | 23:BB:584:C:H6    | 1.85                     | 0.41              |
| 23:BB:1139:G:H5'   | 31:BJ:104:ALA:HB1 | 2.02                     | 0.41              |
| 23:BB:1601:G:H2'   | 23:BB:1602:U:O4'  | 2.20                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:1949:G:H2'   | 23:BB:1950:G:C8    | 2.55                     | 0.41              |
| 23:BB:2104:C:OP1   | 23:BB:2104:C:H4'   | 2.20                     | 0.41              |
| 23:BB:2250:G:H21   | 23:BB:2496:C:H4'   | 1.85                     | 0.41              |
| 23:BB:2491:U:H5''  | 23:BB:2570:G:H5'   | 2.00                     | 0.41              |
| 23:BB:2665:A:H2'   | 23:BB:2666:C:O2    | 2.21                     | 0.41              |
| 23:BB:2675:A:O2'   | 23:BB:2676:C:H5'   | 2.20                     | 0.41              |
| 23:BB:2788:C:H2'   | 23:BB:2789:C:C6    | 2.55                     | 0.41              |
| 25:BC:132:ARG:C    | 25:BC:134:ILE:H    | 2.28                     | 0.41              |
| 26:BD:133:THR:CG2  | 26:BD:134:HIS:N    | 2.83                     | 0.41              |
| 27:BE:38:GLY:C     | 27:BE:40:ARG:N     | 2.75                     | 0.41              |
| 27:BE:149:ILE:HG23 | 27:BE:183:PHE:CG   | 2.56                     | 0.41              |
| 27:BE:152:GLU:C    | 27:BE:153:LEU:HD12 | 2.46                     | 0.41              |
| 27:BE:170:ARG:HH11 | 27:BE:170:ARG:HG2  | 1.85                     | 0.41              |
| 28:BF:173:ASP:O    | 28:BF:173:ASP:CG   | 2.64                     | 0.41              |
| 30:BH:44:ILE:O     | 30:BH:47:PHE:HD2   | 2.04                     | 0.41              |
| 31:BJ:41:LYS:HD2   | 31:BJ:44:TYR:CB    | 2.47                     | 0.41              |
| 32:BK:38:ILE:HA    | 32:BK:60:ALA:O     | 2.20                     | 0.41              |
| 35:BN:24:MET:CE    | 35:BN:44:LEU:HD13  | 2.50                     | 0.41              |
| 37:BP:92:ARG:N     | 37:BP:113:LEU:HD23 | 2.35                     | 0.41              |
| 38:BQ:12:ARG:O     | 38:BQ:15:LYS:HB3   | 2.20                     | 0.41              |
| 41:BT:31:VAL:O     | 41:BT:83:ALA:O     | 2.38                     | 0.41              |
| 41:BT:54:GLU:HB2   | 41:BT:91:GLN:HE22  | 1.85                     | 0.41              |
| 50:B3:23:HIS:HB2   | 50:B3:24:LYS:H     | 1.66                     | 0.41              |
| 50:B3:23:HIS:HE1   | 50:B3:51:LYS:HE2   | 1.84                     | 0.41              |
| 1:CA:42:G:O2'      | 1:CA:43:C:H5'      | 2.20                     | 0.41              |
| 1:CA:191:G:H2'     | 1:CA:192:A:H8      | 1.85                     | 0.41              |
| 1:CA:343:U:O2'     | 1:CA:344:A:H2'     | 2.20                     | 0.41              |
| 1:CA:489:C:H2'     | 1:CA:490:C:H6      | 1.86                     | 0.41              |
| 1:CA:601:G:O2'     | 1:CA:602:A:H5'     | 2.21                     | 0.41              |
| 1:CA:1162:C:H2'    | 1:CA:1163:A:H8     | 1.83                     | 0.41              |
| 1:CA:1187:G:H3'    | 1:CA:1188:A:H8     | 1.86                     | 0.41              |
| 1:CA:1206:G:H2'    | 1:CA:1207:G:O4'    | 2.20                     | 0.41              |
| 1:CA:1469:C:H2'    | 1:CA:1470:U:O4'    | 2.19                     | 0.41              |
| 2:CC:22:PHE:CZ     | 9:CJ:11:LYS:HB3    | 2.55                     | 0.41              |
| 2:CC:70:ALA:C      | 2:CC:105:VAL:HG22  | 2.45                     | 0.41              |
| 3:CD:18:LEU:HD11   | 3:CD:59:LYS:HG3    | 2.02                     | 0.41              |
| 4:CE:37:VAL:HA     | 4:CE:46:GLY:O      | 2.21                     | 0.41              |
| 4:CE:59:ILE:C      | 4:CE:61:LYS:N      | 2.78                     | 0.41              |
| 7:CH:4:ASP:OD1     | 7:CH:76:ARG:NH1    | 2.54                     | 0.41              |
| 7:CH:72:GLU:O      | 7:CH:73:SER:HB2    | 2.20                     | 0.41              |
| 8:CI:30:ASN:HD21   | 8:CI:66:VAL:N      | 2.18                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:CJ:32:THR:HG23  | 9:CJ:33:GLY:N      | 2.31                     | 0.41              |
| 9:CJ:66:GLU:O     | 13:CN:95:LEU:HA    | 2.20                     | 0.41              |
| 13:CN:56:PRO:HG2  | 13:CN:57:SER:H     | 1.85                     | 0.41              |
| 15:CP:52:LEU:O    | 15:CP:53:ASP:C     | 2.62                     | 0.41              |
| 17:CR:62:ARG:HB3  | 17:CR:69:TYR:CE1   | 2.56                     | 0.41              |
| 18:CS:44:ILE:HG23 | 18:CS:62:THR:O     | 2.21                     | 0.41              |
| 19:CT:5:SER:C     | 19:CT:7:LYS:N      | 2.78                     | 0.41              |
| 19:CT:43:LYS:HD3  | 19:CT:86:ALA:HB1   | 2.03                     | 0.41              |
| 20:CB:205:ALA:HB3 | 20:CB:208:ALA:CB   | 2.50                     | 0.41              |
| 22:DA:55:U:H4'    | 28:DF:23:SER:OG    | 2.20                     | 0.41              |
| 23:DB:123:G:H2'   | 23:DB:124:G:C8     | 2.55                     | 0.41              |
| 23:DB:532:A:H5''  | 38:DQ:27:ARG:NH1   | 2.34                     | 0.41              |
| 23:DB:533:G:C5'   | 38:DQ:23:TYR:CD1   | 3.02                     | 0.41              |
| 23:DB:787:C:H3'   | 23:DB:791:C:H41    | 1.85                     | 0.41              |
| 23:DB:941:A:H2'   | 23:DB:942:G:C8     | 2.55                     | 0.41              |
| 23:DB:1220:G:O2'  | 23:DB:1221:C:H5'   | 2.19                     | 0.41              |
| 23:DB:1306:C:H2'  | 23:DB:1307:A:H8    | 1.84                     | 0.41              |
| 23:DB:1341:G:H2'  | 23:DB:1397:U:HO2'  | 1.85                     | 0.41              |
| 23:DB:1399:C:H2'  | 23:DB:1400:U:H6    | 1.83                     | 0.41              |
| 23:DB:1736:U:H2'  | 23:DB:1737:G:O4'   | 2.21                     | 0.41              |
| 23:DB:1789:A:H5'  | 25:DC:220:ARG:NH2  | 2.35                     | 0.41              |
| 23:DB:1795:C:H2'  | 23:DB:1796:U:H6    | 1.85                     | 0.41              |
| 23:DB:2094:A:OP1  | 30:DH:22:LYS:HG3   | 2.21                     | 0.41              |
| 23:DB:2251:G:H8   | 23:DB:2251:G:OP2   | 2.03                     | 0.41              |
| 23:DB:2354:C:O2'  | 43:DW:31:LEU:HG    | 2.20                     | 0.41              |
| 23:DB:2675:A:O2'  | 23:DB:2676:C:H5'   | 2.21                     | 0.41              |
| 23:DB:2682:A:H1'  | 26:DD:22:ILE:HD13  | 2.02                     | 0.41              |
| 23:DB:2788:C:H2'  | 23:DB:2789:C:C6    | 2.55                     | 0.41              |
| 25:DC:21:PRO:O    | 25:DC:22:GLU:CB    | 2.67                     | 0.41              |
| 25:DC:45:ASN:O    | 25:DC:46:GLY:C     | 2.64                     | 0.41              |
| 25:DC:162:GLN:NE2 | 25:DC:174:ARG:NH2  | 2.68                     | 0.41              |
| 26:DD:106:LYS:O   | 26:DD:206:ALA:HB2  | 2.20                     | 0.41              |
| 31:DJ:4:PHE:HB2   | 31:DJ:5:THR:H      | 1.49                     | 0.41              |
| 33:DL:38:GLN:HB2  | 33:DL:39:LYS:H     | 1.66                     | 0.41              |
| 33:DL:135:ILE:N   | 33:DL:135:ILE:HD13 | 2.34                     | 0.41              |
| 35:DN:12:ARG:NH1  | 35:DN:16:HIS:HD2   | 2.18                     | 0.41              |
| 35:DN:86:ARG:NH1  | 35:DN:94:TYR:OH    | 2.53                     | 0.41              |
| 40:DS:7:HIS:O     | 40:DS:8:ARG:HB2    | 2.20                     | 0.41              |
| 40:DS:41:LYS:O    | 40:DS:42:LYS:C     | 2.63                     | 0.41              |
| 40:DS:75:PHE:O    | 40:DS:103:ILE:O    | 2.37                     | 0.41              |
| 41:DT:48:GLN:CG   | 41:DT:49:LYS:N     | 2.84                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:DU:27:VAL:CG1   | 42:DU:33:VAL:HG22  | 2.50                     | 0.41              |
| 42:DU:69:VAL:CG1   | 42:DU:77:GLY:HA2   | 2.50                     | 0.41              |
| 43:DW:74:LYS:HB3   | 43:DW:75:ASN:H     | 1.55                     | 0.41              |
| 1:AA:177:G:P       | 19:AT:59:ARG:HE    | 2.43                     | 0.41              |
| 1:AA:255:G:H1'     | 16:AQ:17:GLU:OE1   | 2.20                     | 0.41              |
| 1:AA:285:C:H2'     | 1:AA:286:C:C6      | 2.56                     | 0.41              |
| 1:AA:313:A:H2'     | 1:AA:314:C:H6      | 1.82                     | 0.41              |
| 1:AA:596:A:O2'     | 1:AA:597:G:H5'     | 2.20                     | 0.41              |
| 1:AA:746:A:H2'     | 1:AA:747:A:H8      | 1.86                     | 0.41              |
| 1:AA:1085:U:H3'    | 1:AA:1086:U:H5     | 1.86                     | 0.41              |
| 1:AA:1179:A:O2'    | 1:AA:1180:A:H5'    | 2.20                     | 0.41              |
| 1:AA:1263:C:H2'    | 1:AA:1264:U:C6     | 2.55                     | 0.41              |
| 1:AA:1350:A:H2'    | 1:AA:1351:U:C6     | 2.55                     | 0.41              |
| 1:AA:1494:G:H2'    | 1:AA:1495:U:C6     | 2.54                     | 0.41              |
| 2:AC:139:ASN:C     | 2:AC:141:MET:N     | 2.78                     | 0.41              |
| 2:AC:179:ALA:HB1   | 2:AC:202:PHE:CE1   | 2.40                     | 0.41              |
| 4:AE:17:VAL:HB     | 4:AE:34:ALA:HB2    | 2.03                     | 0.41              |
| 4:AE:45:VAL:HG23   | 4:AE:71:ILE:CG2    | 2.50                     | 0.41              |
| 6:AG:142:ARG:NH1   | 6:AG:142:ARG:HB2   | 2.35                     | 0.41              |
| 7:AH:87:ARG:O      | 7:AH:91:LEU:HG     | 2.21                     | 0.41              |
| 8:AI:84:ARG:NH1    | 8:AI:84:ARG:HG2    | 2.34                     | 0.41              |
| 9:AJ:48:ARG:HG2    | 9:AJ:48:ARG:NH1    | 2.35                     | 0.41              |
| 9:AJ:88:MET:HE3    | 9:AJ:88:MET:N      | 2.35                     | 0.41              |
| 11:AL:120:ARG:HG3  | 11:AL:120:ARG:NH1  | 2.36                     | 0.41              |
| 14:AO:57:ARG:HH11  | 14:AO:57:ARG:HG3   | 1.85                     | 0.41              |
| 15:AP:6:LEU:CD1    | 15:AP:71:VAL:HB    | 2.51                     | 0.41              |
| 20:AB:162:VAL:HG13 | 20:AB:184:ALA:CB   | 2.47                     | 0.41              |
| 21:AU:36:PHE:HB3   | 21:AU:40:PRO:HG3   | 2.00                     | 0.41              |
| 23:BB:289:G:H2'    | 23:BB:290:U:O4'    | 2.21                     | 0.41              |
| 23:BB:1107:G:O2'   | 23:BB:1108:U:H5'   | 2.20                     | 0.41              |
| 23:BB:1797:G:P     | 25:BC:251:THR:HG23 | 2.60                     | 0.41              |
| 23:BB:2386:A:H2'   | 23:BB:2387:U:H6    | 1.82                     | 0.41              |
| 23:BB:2389:G:H5''  | 23:BB:2390:U:O4'   | 2.20                     | 0.41              |
| 23:BB:2425:A:H4'   | 23:BB:2426:A:OP2   | 2.19                     | 0.41              |
| 23:BB:2527:C:O2'   | 51:B4:1:MET:HA     | 2.20                     | 0.41              |
| 23:BB:2693:G:H21   | 37:BP:95:LYS:NZ    | 2.18                     | 0.41              |
| 25:BC:52:HIS:CD2   | 25:BC:53:ILE:HG13  | 2.56                     | 0.41              |
| 25:BC:73:ILE:HD12  | 25:BC:73:ILE:N     | 2.35                     | 0.41              |
| 26:BD:118:PHE:CA   | 26:BD:164:GLN:HG3  | 2.50                     | 0.41              |
| 26:BD:124:ARG:NH2  | 26:BD:163:GLY:HA3  | 2.35                     | 0.41              |
| 27:BE:6:LYS:NZ     | 27:BE:119:ILE:H    | 2.18                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BE:48:THR:CG2  | 27:BE:86:ALA:HB1   | 2.50                     | 0.41              |
| 27:BE:141:MET:HB2 | 27:BE:143:LEU:HD22 | 2.02                     | 0.41              |
| 27:BE:198:GLU:C   | 27:BE:200:LEU:N    | 2.77                     | 0.41              |
| 28:BF:56:LEU:O    | 28:BF:56:LEU:HD23  | 2.20                     | 0.41              |
| 28:BF:146:ASP:O   | 28:BF:147:ARG:C    | 2.63                     | 0.41              |
| 30:BH:51:ARG:C    | 30:BH:53:GLU:H     | 2.28                     | 0.41              |
| 32:BK:34:GLY:O    | 32:BK:36:GLY:N     | 2.53                     | 0.41              |
| 32:BK:87:LEU:CA   | 32:BK:95:ILE:HG22  | 2.50                     | 0.41              |
| 32:BK:119:ALA:O   | 32:BK:121:GLU:N    | 2.53                     | 0.41              |
| 33:BL:57:LEU:C    | 33:BL:59:ARG:N     | 2.78                     | 0.41              |
| 33:BL:78:ARG:HH21 | 33:BL:82:LEU:HB2   | 1.83                     | 0.41              |
| 34:BM:13:HIS:O    | 34:BM:14:LYS:HB3   | 2.21                     | 0.41              |
| 35:BN:1:MET:HE3   | 35:BN:3:HIS:O      | 2.20                     | 0.41              |
| 38:BQ:50:ARG:C    | 38:BQ:53:LYS:HD3   | 2.46                     | 0.41              |
| 38:BQ:59:LEU:O    | 38:BQ:62:ALA:HB3   | 2.19                     | 0.41              |
| 38:BQ:60:TRP:CE2  | 38:BQ:93:ILE:HA    | 2.54                     | 0.41              |
| 39:BR:31:GLU:HB3  | 39:BR:32:THR:H     | 1.53                     | 0.41              |
| 40:BS:12:SER:O    | 40:BS:16:LYS:HB2   | 2.21                     | 0.41              |
| 41:BT:50:LEU:C    | 41:BT:52:GLU:N     | 2.79                     | 0.41              |
| 42:BU:96:LYS:C    | 42:BU:98:ASN:H     | 2.29                     | 0.41              |
| 46:BZ:3:LYS:O     | 46:BZ:3:LYS:HG3    | 2.19                     | 0.41              |
| 49:B2:3:ARG:O     | 49:B2:5:PHE:N      | 2.53                     | 0.41              |
| 51:B4:33:HIS:CD2  | 51:B4:33:HIS:N     | 2.79                     | 0.41              |
| 1:CA:107:G:C2'    | 1:CA:108:G:H5''    | 2.50                     | 0.41              |
| 1:CA:285:C:H2'    | 1:CA:286:C:C6      | 2.55                     | 0.41              |
| 1:CA:580:C:H2'    | 1:CA:581:G:O4'     | 2.21                     | 0.41              |
| 1:CA:605:U:H2'    | 1:CA:606:G:H8      | 1.86                     | 0.41              |
| 1:CA:664:G:N2     | 1:CA:741:G:H1      | 2.03                     | 0.41              |
| 1:CA:813:U:O2'    | 1:CA:814:A:H5'     | 2.20                     | 0.41              |
| 1:CA:868:C:H2'    | 1:CA:869:G:O4'     | 2.20                     | 0.41              |
| 1:CA:1180:A:OP1   | 8:CI:104:THR:HG23  | 2.21                     | 0.41              |
| 1:CA:1184:G:C2    | 1:CA:1185:G:C8     | 3.07                     | 0.41              |
| 1:CA:1220:G:P     | 13:CN:52:ARG:HH22  | 2.43                     | 0.41              |
| 1:CA:1413:A:O2'   | 1:CA:1414:U:H5'    | 2.20                     | 0.41              |
| 1:CA:1434:A:H2'   | 1:CA:1435:G:O4'    | 2.21                     | 0.41              |
| 2:CC:143:LEU:HB2  | 2:CC:144:GLY:H     | 1.67                     | 0.41              |
| 3:CD:3:TYR:C      | 3:CD:5:GLY:H       | 2.28                     | 0.41              |
| 3:CD:27:ILE:HG22  | 3:CD:27:ILE:O      | 2.20                     | 0.41              |
| 3:CD:74:TYR:CD1   | 3:CD:92:LEU:HD12   | 2.55                     | 0.41              |
| 3:CD:157:ALA:HA   | 3:CD:160:LEU:CD1   | 2.47                     | 0.41              |
| 3:CD:195:ASN:HB3  | 3:CD:197:HIS:NE2   | 2.35                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 6:CG:16:LYS:HB3    | 6:CG:17:PHE:CD1   | 2.54                     | 0.41              |
| 6:CG:43:TYR:O      | 6:CG:44:SER:C     | 2.64                     | 0.41              |
| 8:CI:98:ARG:HA     | 8:CI:103:VAL:CG2  | 2.45                     | 0.41              |
| 9:CJ:83:THR:HG23   | 9:CJ:87:LEU:HD23  | 2.01                     | 0.41              |
| 13:CN:50:LEU:N     | 13:CN:51:PRO:CD   | 2.68                     | 0.41              |
| 23:DB:491:G:C2     | 23:DB:492:A:H1'   | 2.55                     | 0.41              |
| 23:DB:853:C:H2'    | 23:DB:854:C:C6    | 2.54                     | 0.41              |
| 23:DB:1099:G:P     | 52:DI:3:LYS:CA    | 2.95                     | 0.41              |
| 23:DB:1372:U:H2'   | 23:DB:1373:A:H8   | 1.85                     | 0.41              |
| 23:DB:1601:G:H2'   | 23:DB:1602:U:O4'  | 2.20                     | 0.41              |
| 23:DB:1612:C:O3'   | 49:D2:5:PHE:HD2   | 2.02                     | 0.41              |
| 23:DB:1637:A:H5'   | 23:DB:1760:C:O2'  | 2.20                     | 0.41              |
| 23:DB:1685:C:H2'   | 23:DB:1686:C:C6   | 2.55                     | 0.41              |
| 23:DB:1949:G:H2'   | 23:DB:1950:G:C8   | 2.55                     | 0.41              |
| 23:DB:1998:A:H2'   | 23:DB:1999:C:C6   | 2.55                     | 0.41              |
| 23:DB:2026:U:C2    | 23:DB:2027:G:C8   | 3.07                     | 0.41              |
| 23:DB:2228:G:OP1   | 25:DC:257:ARG:HB2 | 2.20                     | 0.41              |
| 23:DB:2321:U:O2    | 23:DB:2321:U:H5'' | 2.19                     | 0.41              |
| 23:DB:2641:G:H5''  | 31:DJ:78:THR:HB   | 2.01                     | 0.41              |
| 23:DB:2849:U:N3    | 23:DB:2867:G:H1'  | 2.35                     | 0.41              |
| 23:DB:2884:U:N3    | 47:D0:48:TYR:CE1  | 2.88                     | 0.41              |
| 25:DC:10:PRO:CD    | 25:DC:202:ARG:NH2 | 2.80                     | 0.41              |
| 25:DC:143:VAL:HG12 | 25:DC:144:GLU:N   | 2.27                     | 0.41              |
| 25:DC:197:ALA:C    | 25:DC:199:HIS:N   | 2.78                     | 0.41              |
| 25:DC:224:MET:HB3  | 25:DC:225:ASN:H   | 1.70                     | 0.41              |
| 27:DE:108:ILE:HG13 | 27:DE:109:LEU:N   | 2.29                     | 0.41              |
| 27:DE:113:VAL:C    | 27:DE:115:GLN:H   | 2.28                     | 0.41              |
| 28:DF:34:THR:O     | 28:DF:153:ILE:HA  | 2.20                     | 0.41              |
| 28:DF:63:LYS:HD2   | 28:DF:64:PRO:HD2  | 2.02                     | 0.41              |
| 29:DG:36:LEU:HD22  | 29:DG:40:VAL:CG1  | 2.50                     | 0.41              |
| 29:DG:37:ASN:C     | 29:DG:40:VAL:HG23 | 2.46                     | 0.41              |
| 29:DG:95:ALA:HB1   | 29:DG:130:ILE:CD1 | 2.48                     | 0.41              |
| 30:DH:57:LYS:H     | 30:DH:57:LYS:HG3  | 1.60                     | 0.41              |
| 33:DL:90:VAL:O     | 33:DL:90:VAL:HG22 | 2.20                     | 0.41              |
| 33:DL:104:GLN:HB2  | 33:DL:105:ILE:H   | 1.60                     | 0.41              |
| 34:DM:70:ASP:C     | 34:DM:72:PRO:HD2  | 2.46                     | 0.41              |
| 35:DN:36:THR:HG22  | 35:DN:40:LYS:HD2  | 2.02                     | 0.41              |
| 35:DN:49:GLU:N     | 35:DN:50:PRO:HD2  | 2.35                     | 0.41              |
| 36:DO:2:ASP:C      | 36:DO:4:LYS:N     | 2.78                     | 0.41              |
| 36:DO:25:ARG:HB2   | 36:DO:40:ILE:HG12 | 2.03                     | 0.41              |
| 37:DP:91:VAL:CG2   | 37:DP:92:ARG:H    | 2.25                     | 0.41              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 38:DQ:25:GLY:HA2  | 38:DQ:29:ARG:CD    | 2.48                     | 0.41              |
| 38:DQ:89:ILE:H    | 38:DQ:89:ILE:CD1   | 2.30                     | 0.41              |
| 39:DR:47:VAL:HG13 | 39:DR:48:LYS:N     | 2.34                     | 0.41              |
| 40:DS:72:THR:CG2  | 40:DS:106:VAL:HG23 | 2.50                     | 0.41              |
| 43:DW:21:GLY:HA2  | 43:DW:25:PHE:CD1   | 2.54                     | 0.41              |
| 43:DW:42:THR:CB   | 43:DW:75:ASN:ND2   | 2.83                     | 0.41              |
| 45:DY:43:ILE:HA   | 45:DY:46:MET:HB2   | 2.01                     | 0.41              |
| 46:DZ:55:GLY:HA2  | 46:DZ:59:ARG:CB    | 2.31                     | 0.41              |
| 46:DZ:66:ILE:HB   | 46:DZ:67:PRO:CD    | 2.42                     | 0.41              |
| 1:AA:75:G:N1      | 1:AA:96:U:C4       | 2.88                     | 0.41              |
| 1:AA:119:A:H4'    | 1:AA:120:A:O4'     | 2.21                     | 0.41              |
| 1:AA:132:C:H5''   | 19:AT:68:LYS:HD2   | 2.02                     | 0.41              |
| 1:AA:224:U:H2'    | 1:AA:225:C:C6      | 2.56                     | 0.41              |
| 1:AA:600:A:H5''   | 7:AH:88:LYS:HD2    | 2.02                     | 0.41              |
| 1:AA:605:U:H2'    | 1:AA:606:G:H8      | 1.86                     | 0.41              |
| 1:AA:635:A:H2'    | 1:AA:636:U:H6      | 1.85                     | 0.41              |
| 1:AA:813:U:O2'    | 1:AA:814:A:H5'     | 2.20                     | 0.41              |
| 1:AA:830:G:H2'    | 1:AA:831:A:H8      | 1.85                     | 0.41              |
| 1:AA:903:G:H2'    | 1:AA:904:U:C6      | 2.55                     | 0.41              |
| 1:AA:1110:A:H2'   | 1:AA:1111:A:C8     | 2.49                     | 0.41              |
| 1:AA:1157:A:H4'   | 1:AA:1158:C:O5'    | 2.20                     | 0.41              |
| 1:AA:1340:A:O2'   | 1:AA:1341:U:H5'    | 2.20                     | 0.41              |
| 2:AC:18:ASN:O     | 2:AC:55:VAL:HA     | 2.20                     | 0.41              |
| 2:AC:180:ASP:O    | 2:AC:180:ASP:CG    | 2.62                     | 0.41              |
| 3:AD:163:GLN:HB2  | 3:AD:164:ARG:HH12  | 1.82                     | 0.41              |
| 5:AF:34:GLY:C     | 5:AF:35:LYS:HG3    | 2.46                     | 0.41              |
| 11:AL:79:ILE:HD13 | 11:AL:96:THR:HG22  | 2.02                     | 0.41              |
| 18:AS:64:GLU:OE1  | 18:AS:65:MET:HG3   | 2.20                     | 0.41              |
| 19:AT:19:HIS:CE1  | 19:AT:23:ARG:HG3   | 2.55                     | 0.41              |
| 21:AU:40:PRO:HG2  | 21:AU:41:THR:N     | 2.28                     | 0.41              |
| 23:BB:175:G:H2'   | 23:BB:176:A:H8     | 1.83                     | 0.41              |
| 23:BB:299:A:H2    | 23:BB:319:G:N3     | 2.18                     | 0.41              |
| 23:BB:482:A:N6    | 23:BB:506:G:H1'    | 2.35                     | 0.41              |
| 23:BB:527:C:C5'   | 23:BB:2779:U:H3    | 2.34                     | 0.41              |
| 23:BB:730:A:H3'   | 55:BB:3597:HOH:O   | 2.19                     | 0.41              |
| 23:BB:778:G:C5'   | 25:BC:48:ILE:HD12  | 2.51                     | 0.41              |
| 23:BB:795:C:H2'   | 23:BB:796:C:C6     | 2.55                     | 0.41              |
| 23:BB:962:G:H2'   | 23:BB:963:U:H6     | 1.85                     | 0.41              |
| 23:BB:1131:G:C1'  | 23:BB:1133:A:H62   | 2.24                     | 0.41              |
| 23:BB:1297:C:OP1  | 23:BB:2710:C:H4'   | 2.20                     | 0.41              |
| 23:BB:1655:A:H2   | 23:BB:2049:G:O3'   | 2.03                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:1841:U:H2'  | 23:BB:1842:G:C8    | 2.55                     | 0.41              |
| 23:BB:1924:C:O2'  | 23:BB:1925:C:H5'   | 2.21                     | 0.41              |
| 23:BB:1998:A:H2'  | 23:BB:1999:C:H6    | 1.84                     | 0.41              |
| 23:BB:2034:U:O2'  | 23:BB:2035:G:H5'   | 2.21                     | 0.41              |
| 23:BB:2185:U:H2'  | 23:BB:2186:G:C8    | 2.51                     | 0.41              |
| 23:BB:2341:G:H2'  | 23:BB:2342:C:C6    | 2.55                     | 0.41              |
| 23:BB:2469:A:C5'  | 34:BM:55:ARG:HG3   | 2.50                     | 0.41              |
| 23:BB:2649:C:O2'  | 23:BB:2650:U:H5'   | 2.19                     | 0.41              |
| 23:BB:2677:G:H2'  | 23:BB:2678:C:C6    | 2.55                     | 0.41              |
| 23:BB:2782:G:O2'  | 23:BB:2783:U:H5'   | 2.20                     | 0.41              |
| 24:BV:51:GLN:NE2  | 24:BV:57:TYR:OH    | 2.53                     | 0.41              |
| 24:BV:79:ARG:C    | 24:BV:87:GLN:HE22  | 2.27                     | 0.41              |
| 25:BC:156:SER:O   | 25:BC:194:VAL:O    | 2.39                     | 0.41              |
| 26:BD:19:GLY:O    | 26:BD:20:VAL:C     | 2.64                     | 0.41              |
| 26:BD:24:VAL:CG2  | 26:BD:193:VAL:HG11 | 2.27                     | 0.41              |
| 27:BE:84:THR:OG1  | 27:BE:85:PHE:N     | 2.53                     | 0.41              |
| 27:BE:114:ARG:H   | 27:BE:114:ARG:HG2  | 1.65                     | 0.41              |
| 27:BE:116:ASP:HB2 | 27:BE:185:LYS:CA   | 2.36                     | 0.41              |
| 28:BF:34:THR:CG2  | 28:BF:89:THR:HG22  | 2.48                     | 0.41              |
| 28:BF:52:ALA:HA   | 28:BF:148:VAL:CG1  | 2.50                     | 0.41              |
| 31:BJ:102:GLU:HG3 | 31:BJ:124:VAL:HG21 | 2.02                     | 0.41              |
| 31:BJ:132:HIS:C   | 31:BJ:134:ALA:N    | 2.78                     | 0.41              |
| 32:BK:33:ALA:CB   | 32:BK:39:ILE:HD11  | 2.50                     | 0.41              |
| 33:BL:6:LEU:HD22  | 33:BL:6:LEU:N      | 2.35                     | 0.41              |
| 33:BL:60:ARG:HD3  | 50:B3:11:LYS:HD2   | 2.02                     | 0.41              |
| 33:BL:123:ARG:O   | 33:BL:124:GLY:C    | 2.63                     | 0.41              |
| 35:BN:9:GLN:HE21  | 35:BN:17:ARG:CZ    | 2.32                     | 0.41              |
| 35:BN:22:ARG:HE   | 35:BN:69:ARG:HE    | 1.67                     | 0.41              |
| 36:BO:20:GLU:O    | 36:BO:21:LEU:C     | 2.63                     | 0.41              |
| 36:BO:76:LYS:HA   | 36:BO:76:LYS:HD2   | 1.95                     | 0.41              |
| 38:BQ:23:TYR:O    | 38:BQ:24:TYR:HB2   | 2.20                     | 0.41              |
| 41:BT:12:ARG:HE   | 44:BX:29:ARG:NH2   | 2.11                     | 0.41              |
| 45:BY:3:THR:O     | 45:BY:6:ILE:HD12   | 2.20                     | 0.41              |
| 46:BZ:58:ASP:HB3  | 46:BZ:63:ARG:HG2   | 2.01                     | 0.41              |
| 51:B4:15:LYS:HD2  | 51:B4:15:LYS:N     | 2.35                     | 0.41              |
| 51:B4:20:ASP:OD2  | 51:B4:20:ASP:C     | 2.63                     | 0.41              |
| 52:BI:2:LYS:HB3   | 52:BI:2:LYS:NZ     | 2.36                     | 0.41              |
| 1:CA:97:G:H3'     | 1:CA:98:A:H8       | 1.85                     | 0.41              |
| 1:CA:224:U:H2'    | 1:CA:225:C:C6      | 2.55                     | 0.41              |
| 1:CA:340:U:H2'    | 1:CA:341:C:C6      | 2.53                     | 0.41              |
| 1:CA:1032:G:H2'   | 1:CA:1033:G:O4'    | 2.20                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:1438:G:O2'    | 1:CA:1439:G:H5'   | 2.20                     | 0.41              |
| 2:CC:4:VAL:HG22    | 2:CC:5:HIS:N      | 2.35                     | 0.41              |
| 3:CD:32:LYS:HG3    | 3:CD:32:LYS:O     | 2.20                     | 0.41              |
| 3:CD:60:VAL:HA     | 3:CD:63:ILE:CG2   | 2.51                     | 0.41              |
| 6:CG:99:ALA:O      | 6:CG:103:ILE:HG13 | 2.20                     | 0.41              |
| 11:CL:18:SER:C     | 11:CL:20:VAL:H    | 2.27                     | 0.41              |
| 13:CN:51:PRO:CG    | 13:CN:52:ARG:H    | 2.30                     | 0.41              |
| 13:CN:89:ARG:HH11  | 13:CN:89:ARG:CB   | 2.34                     | 0.41              |
| 14:CO:80:LEU:CD2   | 14:CO:84:LEU:HD22 | 2.49                     | 0.41              |
| 15:CP:19:VAL:HG13  | 15:CP:37:GLY:C    | 2.45                     | 0.41              |
| 19:CT:66:ILE:HG23  | 19:CT:70:LYS:CG   | 2.51                     | 0.41              |
| 20:CB:72:LYS:HD2   | 20:CB:164:ASP:HB3 | 2.02                     | 0.41              |
| 20:CB:101:THR:HG23 | 20:CB:102:ASN:N   | 2.36                     | 0.41              |
| 22:DA:52:A:H2'     | 22:DA:53:A:C8     | 2.53                     | 0.41              |
| 22:DA:82:U:H5''    | 45:DY:16:LEU:HD11 | 2.03                     | 0.41              |
| 23:DB:247:G:C6     | 50:D3:7:ARG:HD2   | 2.56                     | 0.41              |
| 23:DB:264:C:C2'    | 23:DB:265:A:H5''  | 2.50                     | 0.41              |
| 23:DB:300:A:H2'    | 23:DB:334:C:H1'   | 2.01                     | 0.41              |
| 23:DB:365:U:O5'    | 23:DB:365:U:H6    | 2.02                     | 0.41              |
| 23:DB:484:C:H2'    | 23:DB:485:C:H6    | 1.84                     | 0.41              |
| 23:DB:857:G:H2'    | 23:DB:858:G:C5'   | 2.48                     | 0.41              |
| 23:DB:1023:U:H2'   | 23:DB:1024:G:H5'  | 2.02                     | 0.41              |
| 23:DB:1187:G:H5''  | 39:DR:86:GLN:HE22 | 1.85                     | 0.41              |
| 23:DB:1205:A:H1'   | 23:DB:1206:G:P    | 2.61                     | 0.41              |
| 23:DB:1281:G:H2'   | 23:DB:1282:U:C6   | 2.56                     | 0.41              |
| 23:DB:2073:C:O2'   | 23:DB:2074:U:H5'  | 2.20                     | 0.41              |
| 23:DB:2090:A:C2'   | 46:DZ:49:ARG:NE   | 2.83                     | 0.41              |
| 23:DB:2184:A:H2'   | 23:DB:2185:U:C6   | 2.56                     | 0.41              |
| 23:DB:2273:A:H2'   | 23:DB:2274:A:C8   | 2.56                     | 0.41              |
| 23:DB:2511:U:H6    | 23:DB:2511:U:O5'  | 2.02                     | 0.41              |
| 23:DB:2659:G:N2    | 23:DB:2661:G:H5'' | 2.36                     | 0.41              |
| 23:DB:2677:G:H2'   | 23:DB:2678:C:C6   | 2.55                     | 0.41              |
| 23:DB:2732:G:H3'   | 23:DB:2733:A:H5'  | 2.02                     | 0.41              |
| 25:DC:87:SER:N     | 25:DC:155:ARG:NH1 | 2.68                     | 0.41              |
| 25:DC:252:LYS:HB3  | 25:DC:253:GLY:H   | 1.69                     | 0.41              |
| 26:DD:10:GLY:HA2   | 26:DD:23:PRO:O    | 2.21                     | 0.41              |
| 26:DD:34:VAL:H     | 26:DD:90:PHE:CA   | 2.33                     | 0.41              |
| 27:DE:121:VAL:O    | 27:DE:122:GLU:C   | 2.63                     | 0.41              |
| 28:DF:34:THR:HB    | 28:DF:154:THR:O   | 2.21                     | 0.41              |
| 29:DG:132:LEU:HD12 | 29:DG:132:LEU:O   | 2.20                     | 0.41              |
| 30:DH:113:SER:C    | 30:DH:115:VAL:H   | 2.28                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:DJ:61:LYS:O    | 31:DJ:62:VAL:HG13  | 2.21                     | 0.41              |
| 32:DK:19:VAL:O    | 32:DK:41:ILE:HD11  | 2.20                     | 0.41              |
| 34:DM:35:ALA:HB2  | 34:DM:100:LYS:NZ   | 2.35                     | 0.41              |
| 35:DN:11:ASN:HD22 | 35:DN:11:ASN:HA    | 1.70                     | 0.41              |
| 37:DP:38:ARG:HG3  | 37:DP:39:LEU:N     | 2.20                     | 0.41              |
| 41:DT:66:LYS:HA   | 41:DT:76:ARG:HE    | 1.85                     | 0.41              |
| 41:DT:84:TYR:O    | 41:DT:85:VAL:HG22  | 2.20                     | 0.41              |
| 49:D2:7:PRO:O     | 49:D2:8:SER:CB     | 2.67                     | 0.41              |
| 50:D3:35:LYS:H    | 50:D3:35:LYS:HG3   | 1.70                     | 0.41              |
| 52:DI:100:ILE:O   | 52:DI:139:VAL:HG13 | 2.20                     | 0.41              |
| 1:AA:66:A:O2'     | 1:AA:67:C:H5'      | 2.21                     | 0.41              |
| 1:AA:68:G:H5'     | 1:AA:171:A:O2'     | 2.21                     | 0.41              |
| 1:AA:265:G:H4'    | 16:AQ:66:LEU:O     | 2.20                     | 0.41              |
| 1:AA:404:G:H2'    | 1:AA:405:U:H6      | 1.85                     | 0.41              |
| 1:AA:489:C:H2'    | 1:AA:490:C:H6      | 1.86                     | 0.41              |
| 1:AA:551:U:H2'    | 1:AA:552:U:H6      | 1.86                     | 0.41              |
| 1:AA:666:G:H5'    | 1:AA:726:C:H1'     | 2.03                     | 0.41              |
| 1:AA:738:C:H2'    | 1:AA:739:C:H6      | 1.86                     | 0.41              |
| 1:AA:1005:A:O2'   | 1:AA:1006:G:H5'    | 2.21                     | 0.41              |
| 1:AA:1347:G:N2    | 1:AA:1373:G:H2'    | 2.35                     | 0.41              |
| 1:AA:1370:G:O2'   | 1:AA:1371:G:H5'    | 2.20                     | 0.41              |
| 1:AA:1395:C:O2    | 1:AA:1395:C:H2'    | 2.21                     | 0.41              |
| 2:AC:7:ASN:OD1    | 2:AC:183:TYR:HB3   | 2.21                     | 0.41              |
| 2:AC:14:VAL:HG23  | 2:AC:15:LYS:HG2    | 2.03                     | 0.41              |
| 2:AC:181:ILE:HG22 | 2:AC:182:ASP:N     | 2.35                     | 0.41              |
| 3:AD:32:LYS:HB3   | 3:AD:35:GLN:CG     | 2.50                     | 0.41              |
| 3:AD:176:LYS:HA   | 3:AD:177:MET:HE2   | 2.02                     | 0.41              |
| 4:AE:95:MET:CE    | 4:AE:114:LEU:HD11  | 2.51                     | 0.41              |
| 4:AE:131:ASN:HD22 | 4:AE:134:ASN:CG    | 2.28                     | 0.41              |
| 6:AG:21:LEU:HG    | 6:AG:22:LEU:H      | 1.84                     | 0.41              |
| 6:AG:22:LEU:O     | 6:AG:26:VAL:HG13   | 2.19                     | 0.41              |
| 7:AH:92:PRO:C     | 7:AH:93:LYS:HD3    | 2.46                     | 0.41              |
| 10:AK:122:PRO:CG  | 21:AU:35:GLU:HG2   | 2.51                     | 0.41              |
| 13:AN:11:LYS:HA   | 13:AN:11:LYS:NZ    | 2.34                     | 0.41              |
| 13:AN:20:PHE:CG   | 13:AN:24:ALA:HB2   | 2.56                     | 0.41              |
| 14:AO:15:GLY:C    | 14:AO:17:ASP:N     | 2.78                     | 0.41              |
| 18:AS:48:ILE:HG22 | 18:AS:49:ALA:N     | 2.35                     | 0.41              |
| 20:AB:45:THR:HA   | 20:AB:48:MET:CG    | 2.51                     | 0.41              |
| 21:AU:33:ARG:CZ   | 21:AU:34:ARG:HG3   | 2.50                     | 0.41              |
| 21:AU:33:ARG:HB3  | 21:AU:34:ARG:H     | 1.64                     | 0.41              |
| 23:BB:15:G:H2'    | 23:BB:16:C:H6      | 1.84                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:466:A:H2    | 23:BB:795:C:O2     | 2.03                     | 0.41              |
| 23:BB:477:A:H2'   | 23:BB:478:A:O4'    | 2.20                     | 0.41              |
| 23:BB:724:U:O2'   | 23:BB:725:G:H5'    | 2.21                     | 0.41              |
| 23:BB:990:A:N3    | 39:BR:79:ARG:NH2   | 2.68                     | 0.41              |
| 23:BB:1281:G:H2'  | 23:BB:1282:U:C6    | 2.56                     | 0.41              |
| 23:BB:1299:G:C5'  | 23:BB:1301:A:H1'   | 2.51                     | 0.41              |
| 23:BB:1498:C:H2'  | 23:BB:1499:C:H6    | 1.86                     | 0.41              |
| 23:BB:2198:A:N6   | 30:BH:25:TYR:HE1   | 2.18                     | 0.41              |
| 23:BB:2385:C:H2'  | 23:BB:2386:A:H8    | 1.86                     | 0.41              |
| 23:BB:2457:U:C2'  | 23:BB:2458:G:H5'   | 2.49                     | 0.41              |
| 23:BB:2710:C:H2'  | 23:BB:2711:A:C8    | 2.56                     | 0.41              |
| 23:BB:2825:G:C2'  | 23:BB:2826:A:H5'   | 2.51                     | 0.41              |
| 25:BC:265:PHE:HB3 | 25:BC:266:ILE:H    | 1.74                     | 0.41              |
| 26:BD:109:VAL:O   | 26:BD:172:VAL:HG22 | 2.21                     | 0.41              |
| 28:BF:87:LYS:O    | 28:BF:88:VAL:HB    | 2.20                     | 0.41              |
| 28:BF:133:GLU:OE1 | 28:BF:150:GLY:N    | 2.53                     | 0.41              |
| 29:BG:29:ASN:N    | 29:BG:29:ASN:ND2   | 2.68                     | 0.41              |
| 30:BH:31:VAL:HG22 | 30:BH:37:VAL:HG22  | 2.02                     | 0.41              |
| 31:BJ:109:LEU:O   | 31:BJ:111:LYS:HG3  | 2.21                     | 0.41              |
| 32:BK:20:MET:HB3  | 32:BK:42:THR:HB    | 2.01                     | 0.41              |
| 33:BL:21:ARG:HB3  | 33:BL:21:ARG:CZ    | 2.50                     | 0.41              |
| 33:BL:60:ARG:O    | 33:BL:60:ARG:HG3   | 2.20                     | 0.41              |
| 41:BT:70:HIS:CG   | 41:BT:74:ILE:HB    | 2.55                     | 0.41              |
| 45:BY:24:LEU:HD23 | 45:BY:29:ARG:HH22  | 1.85                     | 0.41              |
| 46:BZ:64:PHE:C    | 46:BZ:66:ILE:H     | 2.27                     | 0.41              |
| 47:B0:32:THR:HG21 | 47:B0:35:GLU:HB3   | 2.02                     | 0.41              |
| 49:B2:21:ARG:CB   | 49:B2:31:LEU:HD21  | 2.49                     | 0.41              |
| 51:B4:7:VAL:HB    | 51:B4:35:GLN:HE21  | 1.85                     | 0.41              |
| 1:CA:79:G:H2'     | 1:CA:80:A:H8       | 1.83                     | 0.41              |
| 1:CA:371:A:H2'    | 1:CA:372:C:C6      | 2.54                     | 0.41              |
| 1:CA:644:U:O2'    | 1:CA:645:G:H5'     | 2.20                     | 0.41              |
| 1:CA:828:U:O2'    | 20:CB:24:PRO:HB3   | 2.20                     | 0.41              |
| 1:CA:1133:G:H2'   | 1:CA:1134:G:O4'    | 2.21                     | 0.41              |
| 1:CA:1363:A:O2'   | 1:CA:1365:G:N7     | 2.45                     | 0.41              |
| 3:CD:93:LEU:HA    | 3:CD:96:ARG:HG3    | 2.03                     | 0.41              |
| 3:CD:158:LEU:CD1  | 3:CD:177:MET:HG2   | 2.50                     | 0.41              |
| 3:CD:183:ARG:HD2  | 3:CD:183:ARG:C     | 2.45                     | 0.41              |
| 8:CI:15:ALA:O     | 8:CI:66:VAL:HA     | 2.21                     | 0.41              |
| 9:CJ:57:VAL:HG22  | 9:CJ:58:ASN:N      | 2.26                     | 0.41              |
| 10:CK:82:GLU:HB3  | 10:CK:108:ASN:HB3  | 2.02                     | 0.41              |
| 11:CL:29:LYS:O    | 11:CL:81:ILE:N     | 2.50                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:CO:2:LEU:O      | 14:CO:3:SER:HB3    | 2.18                     | 0.41              |
| 14:CO:30:LEU:O     | 14:CO:34:GLN:HG3   | 2.20                     | 0.41              |
| 19:CT:79:THR:C     | 19:CT:81:GLN:H     | 2.29                     | 0.41              |
| 23:DB:179:C:OP1    | 49:D2:28:ARG:HD3   | 2.18                     | 0.41              |
| 23:DB:281:C:H2'    | 23:DB:282:A:C8     | 2.56                     | 0.41              |
| 23:DB:374:A:H2'    | 23:DB:375:G:O4'    | 2.21                     | 0.41              |
| 23:DB:866:A:N1     | 23:DB:913:U:H4'    | 2.36                     | 0.41              |
| 23:DB:928:A:H1'    | 45:DY:1:ALA:CA     | 2.48                     | 0.41              |
| 23:DB:1345:C:H5'   | 23:DB:1396:U:H5    | 1.85                     | 0.41              |
| 23:DB:1394:U:O2'   | 23:DB:1395:A:H5'   | 2.21                     | 0.41              |
| 23:DB:1434:A:H4'   | 23:DB:1434:A:OP1   | 2.20                     | 0.41              |
| 23:DB:1903:G:OP1   | 25:DC:239:PHE:CD2  | 2.74                     | 0.41              |
| 23:DB:1977:A:H2'   | 23:DB:1978:A:O4'   | 2.21                     | 0.41              |
| 23:DB:2032:G:N2    | 26:DD:150:GLN:HB3  | 2.36                     | 0.41              |
| 23:DB:2034:U:O2'   | 23:DB:2035:G:H5'   | 2.20                     | 0.41              |
| 23:DB:2070:A:H2'   | 23:DB:2071:A:O4'   | 2.20                     | 0.41              |
| 23:DB:2072:C:H2'   | 23:DB:2073:C:C6    | 2.54                     | 0.41              |
| 23:DB:2092:U:H5    | 23:DB:2226:C:OP2   | 2.02                     | 0.41              |
| 23:DB:2101:A:O2'   | 23:DB:2102:G:H5'   | 2.21                     | 0.41              |
| 23:DB:2204:G:C5'   | 25:DC:149:LYS:HE3  | 2.50                     | 0.41              |
| 23:DB:2642:G:H5''  | 31:DJ:80:HIS:HB2   | 2.02                     | 0.41              |
| 23:DB:2849:U:O4'   | 23:DB:2868:A:C6    | 2.73                     | 0.41              |
| 25:DC:160:TYR:CE2  | 25:DC:193:GLU:HG2  | 2.56                     | 0.41              |
| 27:DE:135:ALA:O    | 27:DE:139:LYS:N    | 2.53                     | 0.41              |
| 28:DF:136:ILE:HG22 | 28:DF:137:PHE:N    | 2.35                     | 0.41              |
| 29:DG:104:LEU:HD12 | 29:DG:106:LEU:HD21 | 2.02                     | 0.41              |
| 30:DH:127:GLU:HB2  | 30:DH:143:ILE:CG2  | 2.50                     | 0.41              |
| 31:DJ:38:GLY:O     | 31:DJ:41:LYS:HD3   | 2.21                     | 0.41              |
| 31:DJ:48:VAL:HG12  | 31:DJ:49:ASP:N     | 2.35                     | 0.41              |
| 31:DJ:58:ASN:C     | 31:DJ:60:ASP:N     | 2.78                     | 0.41              |
| 33:DL:143:GLU:HG2  | 33:DL:143:GLU:O    | 2.20                     | 0.41              |
| 34:DM:71:LYS:HZ3   | 34:DM:71:LYS:CA    | 2.29                     | 0.41              |
| 34:DM:129:THR:O    | 34:DM:131:VAL:HG12 | 2.20                     | 0.41              |
| 35:DN:72:ASP:OD2   | 35:DN:75:ILE:HG23  | 2.20                     | 0.41              |
| 35:DN:75:ILE:HG13  | 35:DN:76:VAL:N     | 2.36                     | 0.41              |
| 36:DO:26:LEU:HD22  | 36:DO:93:ASP:HA    | 2.02                     | 0.41              |
| 37:DP:50:ARG:HH11  | 37:DP:50:ARG:CB    | 2.31                     | 0.41              |
| 39:DR:18:GLN:O     | 39:DR:19:THR:HG23  | 2.19                     | 0.41              |
| 39:DR:27:ILE:O     | 39:DR:27:ILE:HG23  | 2.20                     | 0.41              |
| 42:DU:42:LYS:N     | 42:DU:57:ILE:HD12  | 2.28                     | 0.41              |
| 43:DW:3:LYS:HA     | 43:DW:3:LYS:HZ2    | 1.79                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 45:DY:2:LYS:H     | 45:DY:37:ARG:HB2  | 1.83                     | 0.41              |
| 46:DZ:28:VAL:HG23 | 46:DZ:29:GLY:H    | 1.85                     | 0.41              |
| 46:DZ:34:LEU:HB3  | 46:DZ:35:ASP:H    | 1.54                     | 0.41              |
| 47:D0:26:SER:C    | 47:D0:38:LEU:HD21 | 2.44                     | 0.41              |
| 51:D4:2:LYS:HG2   | 51:D4:37:GLN:C    | 2.46                     | 0.41              |
| 1:AA:91:U:C4      | 1:AA:92:U:C4      | 3.09                     | 0.41              |
| 1:AA:92:U:O2'     | 1:AA:93:U:H5'     | 2.20                     | 0.41              |
| 1:AA:407:U:H3'    | 1:AA:408:A:H8     | 1.85                     | 0.41              |
| 1:AA:878:A:H2'    | 1:AA:879:C:C6     | 2.56                     | 0.41              |
| 1:AA:989:U:H2'    | 1:AA:990:C:H6     | 1.85                     | 0.41              |
| 1:AA:1217:C:H2'   | 1:AA:1218:C:C6    | 2.55                     | 0.41              |
| 1:AA:1300:G:C2'   | 1:AA:1301:U:OP2   | 2.69                     | 0.41              |
| 1:AA:1457:G:H2'   | 1:AA:1458:G:H8    | 1.86                     | 0.41              |
| 2:AC:35:ASP:O     | 2:AC:38:VAL:HG22  | 2.21                     | 0.41              |
| 2:AC:86:LEU:O     | 2:AC:90:VAL:HG22  | 2.20                     | 0.41              |
| 3:AD:109:THR:HG23 | 3:AD:112:GLU:H    | 1.86                     | 0.41              |
| 6:AG:10:LYS:HB2   | 6:AG:10:LYS:NZ    | 2.36                     | 0.41              |
| 10:AK:95:THR:HG23 | 10:AK:96:ILE:HG13 | 2.01                     | 0.41              |
| 14:AO:58:MET:HG2  | 14:AO:58:MET:H    | 1.68                     | 0.41              |
| 15:AP:40:ASN:HD21 | 15:AP:42:ILE:CG1  | 2.33                     | 0.41              |
| 18:AS:40:PHE:CG   | 18:AS:41:PRO:HD2  | 2.56                     | 0.41              |
| 19:AT:54:GLN:N    | 19:AT:55:PRO:CD   | 2.82                     | 0.41              |
| 20:AB:76:SER:OG   | 20:AB:92:ASN:HB2  | 2.21                     | 0.41              |
| 22:BA:12:C:H41    | 43:BW:50:VAL:HG23 | 1.86                     | 0.41              |
| 22:BA:81:G:H2'    | 22:BA:82:U:C6     | 2.55                     | 0.41              |
| 23:BB:32:C:H5'    | 23:BB:1238:G:OP1  | 2.19                     | 0.41              |
| 23:BB:484:C:H2'   | 23:BB:485:C:H6    | 1.85                     | 0.41              |
| 23:BB:490:C:H4'   | 23:BB:491:G:OP2   | 2.20                     | 0.41              |
| 23:BB:545:U:C2    | 23:BB:548:G:OP2   | 2.74                     | 0.41              |
| 23:BB:599:A:H2'   | 23:BB:600:G:H8    | 1.84                     | 0.41              |
| 23:BB:1036:G:C6   | 23:BB:1120:G:C6   | 3.07                     | 0.41              |
| 23:BB:1097:U:H2'  | 23:BB:1098:A:C5'  | 2.50                     | 0.41              |
| 23:BB:1133:A:N6   | 23:BB:2025:C:O2'  | 2.54                     | 0.41              |
| 23:BB:1372:U:H2'  | 23:BB:1373:A:C8   | 2.55                     | 0.41              |
| 23:BB:1593:A:H2'  | 23:BB:1594:U:O4'  | 2.20                     | 0.41              |
| 23:BB:1945:G:H2'  | 23:BB:1946:U:H6   | 1.81                     | 0.41              |
| 23:BB:2205:A:H2'  | 23:BB:2206:C:H6   | 1.86                     | 0.41              |
| 23:BB:2270:A:C4'  | 43:BW:18:LYS:HB3  | 2.49                     | 0.41              |
| 23:BB:2372:U:H1'  | 48:B1:45:HIS:CE1  | 2.56                     | 0.41              |
| 23:BB:2659:G:N2   | 23:BB:2661:G:H5'' | 2.36                     | 0.41              |
| 23:BB:2668:G:O2'  | 23:BB:2669:G:H5'  | 2.20                     | 0.41              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:BV:80:HIS:CD2   | 24:BV:81:PRO:HD2  | 2.56                     | 0.41              |
| 26:BD:3:GLY:HA3    | 26:BD:49:GLN:HE22 | 1.86                     | 0.41              |
| 26:BD:138:LEU:HD23 | 26:BD:138:LEU:N   | 2.26                     | 0.41              |
| 26:BD:138:LEU:CD2  | 26:BD:138:LEU:N   | 2.79                     | 0.41              |
| 27:BE:6:LYS:HB2    | 27:BE:12:LEU:HD11 | 2.01                     | 0.41              |
| 27:BE:6:LYS:HZ1    | 27:BE:119:ILE:N   | 2.19                     | 0.41              |
| 27:BE:85:PHE:O     | 27:BE:86:ALA:C    | 2.64                     | 0.41              |
| 28:BF:32:LYS:HD2   | 28:BF:89:THR:HB   | 2.01                     | 0.41              |
| 29:BG:97:VAL:HG21  | 29:BG:123:GLU:HA  | 2.02                     | 0.41              |
| 29:BG:121:THR:C    | 29:BG:133:LYS:HD3 | 2.46                     | 0.41              |
| 31:BJ:102:GLU:HG2  | 31:BJ:103:ILE:N   | 2.35                     | 0.41              |
| 34:BM:69:PRO:HB2   | 34:BM:70:ASP:H    | 1.62                     | 0.41              |
| 35:BN:1:MET:SD     | 35:BN:2:ARG:HB2   | 2.60                     | 0.41              |
| 35:BN:29:VAL:HG22  | 35:BN:83:LEU:CD2  | 2.48                     | 0.41              |
| 35:BN:121:LYS:HB2  | 35:BN:123:GLU:CD  | 2.46                     | 0.41              |
| 38:BQ:80:ASN:HD22  | 38:BQ:80:ASN:HA   | 1.66                     | 0.41              |
| 40:BS:79:GLY:O     | 40:BS:80:PRO:C    | 2.63                     | 0.41              |
| 40:BS:85:ILE:HG22  | 40:BS:86:MET:N    | 2.35                     | 0.41              |
| 44:BX:51:ALA:O     | 44:BX:52:ARG:C    | 2.63                     | 0.41              |
| 45:BY:8:GLN:NE2    | 45:BY:23:LEU:HD21 | 2.35                     | 0.41              |
| 46:BZ:49:ARG:C     | 46:BZ:49:ARG:HD3  | 2.46                     | 0.41              |
| 47:B0:27:LEU:C     | 47:B0:36:LYS:HD3  | 2.45                     | 0.41              |
| 50:B3:34:LYS:HB3   | 50:B3:35:LYS:CE   | 2.50                     | 0.41              |
| 51:B4:10:LEU:O     | 51:B4:11:CYS:HB3  | 2.21                     | 0.41              |
| 52:BI:130:GLY:HA2  | 52:BI:133:ARG:NH2 | 2.35                     | 0.41              |
| 1:CA:162:A:H2'     | 1:CA:163:C:O4'    | 2.20                     | 0.41              |
| 1:CA:207:C:O2'     | 1:CA:208:U:H5'    | 2.20                     | 0.41              |
| 1:CA:596:A:O2'     | 1:CA:597:G:H5'    | 2.20                     | 0.41              |
| 1:CA:688:G:H5'     | 10:CK:48:GLY:CA   | 2.50                     | 0.41              |
| 1:CA:821:G:H2'     | 1:CA:822:U:C6     | 2.55                     | 0.41              |
| 1:CA:857:C:O2'     | 1:CA:858:G:H5'    | 2.21                     | 0.41              |
| 1:CA:928:G:O2'     | 1:CA:929:G:H5'    | 2.20                     | 0.41              |
| 1:CA:1190:G:H5'    | 2:CC:175:HIS:NE2  | 2.36                     | 0.41              |
| 1:CA:1293:C:H2'    | 1:CA:1294:G:O4'   | 2.20                     | 0.41              |
| 2:CC:111:ASP:O     | 2:CC:112:ALA:HB3  | 2.21                     | 0.41              |
| 4:CE:64:GLU:HA     | 4:CE:67:ARG:HH12  | 1.85                     | 0.41              |
| 4:CE:89:THR:HG22   | 4:CE:91:SER:N     | 2.22                     | 0.41              |
| 6:CG:24:LYS:HA     | 6:CG:27:ASN:HD22  | 1.85                     | 0.41              |
| 6:CG:109:LYS:HD3   | 6:CG:109:LYS:C    | 2.46                     | 0.41              |
| 9:CJ:44:THR:HG23   | 9:CJ:70:HIS:HA    | 2.02                     | 0.41              |
| 10:CK:110:THR:HG22 | 21:CU:4:LYS:HA    | 2.02                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:CL:49:ARG:HD3   | 11:CL:89:LEU:HD21  | 2.01                     | 0.41              |
| 17:CR:20:ILE:HD12  | 17:CR:53:GLN:NE2   | 2.34                     | 0.41              |
| 20:CB:116:LEU:HD22 | 20:CB:140:LEU:CD2  | 2.41                     | 0.41              |
| 20:CB:156:LEU:HD11 | 20:CB:178:LEU:CD1  | 2.33                     | 0.41              |
| 20:CB:216:VAL:C    | 20:CB:218:ALA:N    | 2.78                     | 0.41              |
| 23:DB:63:A:H8      | 23:DB:63:A:OP2     | 2.04                     | 0.41              |
| 23:DB:82:U:H2'     | 23:DB:83:A:O4'     | 2.20                     | 0.41              |
| 23:DB:413:C:O5'    | 23:DB:413:C:H6     | 2.04                     | 0.41              |
| 23:DB:432:A:H2'    | 23:DB:433:C:O4'    | 2.20                     | 0.41              |
| 23:DB:523:C:H4'    | 23:DB:540:C:O2     | 2.21                     | 0.41              |
| 23:DB:570:G:C2'    | 23:DB:571:U:H5'    | 2.51                     | 0.41              |
| 23:DB:794:A:C4     | 23:DB:795:C:C5     | 3.09                     | 0.41              |
| 23:DB:811:U:H2'    | 33:DL:32:GLY:HA2   | 2.02                     | 0.41              |
| 23:DB:834:G:H2'    | 23:DB:835:C:C6     | 2.55                     | 0.41              |
| 23:DB:921:C:C2     | 23:DB:922:C:C5     | 3.09                     | 0.41              |
| 23:DB:1064:C:O2'   | 23:DB:1065:U:H5'   | 2.20                     | 0.41              |
| 23:DB:1449:G:H2'   | 23:DB:1450:G:C8    | 2.56                     | 0.41              |
| 23:DB:1460:U:H5''  | 23:DB:1461:C:C6    | 2.56                     | 0.41              |
| 23:DB:1678:A:C2'   | 23:DB:1679:A:H5'   | 2.50                     | 0.41              |
| 23:DB:1893:C:H2'   | 23:DB:1894:C:O4'   | 2.21                     | 0.41              |
| 23:DB:2191:A:H2'   | 23:DB:2192:U:H6    | 1.83                     | 0.41              |
| 23:DB:2221:G:H2'   | 23:DB:2222:C:C6    | 2.56                     | 0.41              |
| 23:DB:2668:G:O2'   | 23:DB:2669:G:H5'   | 2.20                     | 0.41              |
| 23:DB:2681:C:OP2   | 26:DD:114:LYS:HE3  | 2.20                     | 0.41              |
| 23:DB:2686:G:H2'   | 23:DB:2687:U:C6    | 2.55                     | 0.41              |
| 24:DV:48:MET:O     | 24:DV:51:GLN:HG3   | 2.20                     | 0.41              |
| 25:DC:28:PRO:CG    | 25:DC:79:ARG:HE    | 2.34                     | 0.41              |
| 25:DC:59:GLN:HB2   | 25:DC:60:ALA:H     | 1.64                     | 0.41              |
| 25:DC:107:LYS:HD2  | 25:DC:196:ASN:ND2  | 2.36                     | 0.41              |
| 27:DE:15:SER:HB3   | 27:DE:196:VAL:HG13 | 2.02                     | 0.41              |
| 28:DF:23:SER:C     | 28:DF:25:MET:H     | 2.28                     | 0.41              |
| 29:DG:104:LEU:N    | 29:DG:112:VAL:O    | 2.51                     | 0.41              |
| 29:DG:154:GLU:OE2  | 29:DG:159:LYS:HB2  | 2.21                     | 0.41              |
| 30:DH:9:VAL:O      | 30:DH:11:ASN:N     | 2.54                     | 0.41              |
| 31:DJ:84:ILE:CG1   | 31:DJ:85:LYS:H     | 2.33                     | 0.41              |
| 32:DK:99:ILE:O     | 32:DK:119:ALA:HB2  | 2.20                     | 0.41              |
| 34:DM:119:LEU:H    | 34:DM:119:LEU:CD2  | 2.34                     | 0.41              |
| 35:DN:38:LEU:O     | 35:DN:41:ALA:HB3   | 2.21                     | 0.41              |
| 37:DP:61:ARG:O     | 37:DP:62:LYS:C     | 2.64                     | 0.41              |
| 38:DQ:25:GLY:O     | 38:DQ:26:ALA:C     | 2.62                     | 0.41              |
| 39:DR:39:LEU:C     | 39:DR:41:ILE:N     | 2.78                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 39:DR:40:MET:O    | 39:DR:41:ILE:C     | 2.63                     | 0.41              |
| 45:DY:26:LEU:HD23 | 45:DY:26:LEU:N     | 2.35                     | 0.41              |
| 46:DZ:17:SER:H    | 46:DZ:21:VAL:HG12  | 1.85                     | 0.41              |
| 46:DZ:54:GLY:N    | 46:DZ:57:VAL:HG23  | 2.15                     | 0.41              |
| 46:DZ:62:LYS:C    | 46:DZ:65:ASN:HD21  | 2.28                     | 0.41              |
| 52:DI:9:LYS:HG2   | 52:DI:57:VAL:HG22  | 2.03                     | 0.41              |
| 1:AA:42:G:O2'     | 1:AA:43:C:H5'      | 2.20                     | 0.41              |
| 1:AA:102:G:N3     | 1:AA:151:A:H2      | 2.19                     | 0.41              |
| 1:AA:191:G:H2'    | 1:AA:192:A:C8      | 2.56                     | 0.41              |
| 1:AA:191:G:H2'    | 1:AA:192:A:H8      | 1.86                     | 0.41              |
| 1:AA:619:U:C2     | 3:AD:131:ILE:HD12  | 2.56                     | 0.41              |
| 1:AA:857:C:O2'    | 1:AA:858:G:H5'     | 2.21                     | 0.41              |
| 1:AA:967:C:OP1    | 1:AA:969:A:C8      | 2.74                     | 0.41              |
| 1:AA:1010:U:H2'   | 1:AA:1011:C:H6     | 1.86                     | 0.41              |
| 1:AA:1207:G:O2'   | 1:AA:1208:C:H5'    | 2.20                     | 0.41              |
| 1:AA:1221:G:O2'   | 1:AA:1222:G:H5'    | 2.20                     | 0.41              |
| 1:AA:1505:G:H5''  | 1:AA:1506:U:O5'    | 2.21                     | 0.41              |
| 2:AC:38:VAL:CG2   | 2:AC:39:ARG:N      | 2.83                     | 0.41              |
| 4:AE:35:LEU:HD21  | 4:AE:47:PHE:HB2    | 2.02                     | 0.41              |
| 4:AE:89:THR:HG21  | 4:AE:134:ASN:ND2   | 2.36                     | 0.41              |
| 8:AI:12:LYS:N     | 8:AI:109:GLN:HE22  | 2.13                     | 0.41              |
| 10:AK:88:PRO:HA   | 10:AK:92:ARG:CD    | 2.51                     | 0.41              |
| 11:AL:5:GLN:HA    | 11:AL:8:ARG:NE     | 2.35                     | 0.41              |
| 11:AL:113:ARG:HA  | 11:AL:118:VAL:CG2  | 2.51                     | 0.41              |
| 12:AM:12:LYS:CB   | 12:AM:17:ALA:HB2   | 2.51                     | 0.41              |
| 12:AM:12:LYS:HB3  | 12:AM:17:ALA:HB2   | 2.02                     | 0.41              |
| 14:AO:63:ARG:NH1  | 14:AO:63:ARG:HB3   | 2.35                     | 0.41              |
| 15:AP:12:LYS:C    | 15:AP:14:ARG:N     | 2.78                     | 0.41              |
| 18:AS:66:VAL:C    | 18:AS:68:HIS:N     | 2.78                     | 0.41              |
| 23:BB:558:U:C5'   | 31:BJ:114:LEU:HD22 | 2.51                     | 0.41              |
| 23:BB:689:A:H2'   | 23:BB:690:G:H8     | 1.85                     | 0.41              |
| 23:BB:834:G:O2'   | 50:B3:50:SER:HB3   | 2.21                     | 0.41              |
| 23:BB:844:A:C2    | 23:BB:845:A:N1     | 2.89                     | 0.41              |
| 23:BB:967:U:C2    | 23:BB:968:C:C5     | 3.09                     | 0.41              |
| 23:BB:968:C:H4'   | 45:BY:16:LEU:HD23  | 2.03                     | 0.41              |
| 23:BB:989:G:OP1   | 23:BB:1157:G:H4'   | 2.20                     | 0.41              |
| 23:BB:1196:C:H2'  | 23:BB:1197:G:C8    | 2.56                     | 0.41              |
| 23:BB:1434:A:OP1  | 23:BB:1434:A:H4'   | 2.20                     | 0.41              |
| 23:BB:1656:C:OP1  | 26:BD:141:ARG:HD3  | 2.21                     | 0.41              |
| 23:BB:1827:U:C2'  | 23:BB:1828:G:H5'   | 2.51                     | 0.41              |
| 23:BB:2094:A:H5'  | 30:BH:25:TYR:CD1   | 2.54                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:2096:C:H2'   | 23:BB:2097:A:H8    | 1.86                     | 0.41              |
| 23:BB:2467:C:H1'   | 34:BM:118:LYS:HG2  | 2.01                     | 0.41              |
| 23:BB:2512:C:H5''  | 26:BD:125:TRP:CZ3  | 2.56                     | 0.41              |
| 23:BB:2653:U:H2'   | 23:BB:2654:A:C8    | 2.55                     | 0.41              |
| 25:BC:81:GLU:O     | 25:BC:90:ILE:HG22  | 2.21                     | 0.41              |
| 25:BC:90:ILE:HG23  | 25:BC:91:ALA:N     | 2.35                     | 0.41              |
| 26:BD:11:MET:CE    | 37:BP:9:GLN:HG2    | 2.51                     | 0.41              |
| 26:BD:165:MET:CG   | 26:BD:166:GLY:H    | 2.33                     | 0.41              |
| 27:BE:45:ALA:HB3   | 27:BE:89:PRO:HA    | 2.02                     | 0.41              |
| 27:BE:132:LYS:H    | 27:BE:132:LYS:HG3  | 1.55                     | 0.41              |
| 28:BF:36:ASN:HB2   | 28:BF:87:LYS:CA    | 2.33                     | 0.41              |
| 30:BH:141:LYS:HE2  | 30:BH:141:LYS:HB2  | 1.86                     | 0.41              |
| 31:BJ:34:ARG:CG    | 31:BJ:39:LYS:HD2   | 2.50                     | 0.41              |
| 33:BL:4:ASN:O      | 33:BL:6:LEU:HD22   | 2.21                     | 0.41              |
| 33:BL:30:THR:O     | 33:BL:31:GLY:C     | 2.63                     | 0.41              |
| 36:BO:30:ARG:O     | 36:BO:31:THR:O     | 2.39                     | 0.41              |
| 36:BO:60:GLU:HG3   | 36:BO:61:GLN:N     | 2.35                     | 0.41              |
| 36:BO:64:TYR:HD1   | 36:BO:74:VAL:HG21  | 1.84                     | 0.41              |
| 36:BO:103:VAL:HG23 | 36:BO:104:GLN:N    | 2.35                     | 0.41              |
| 37:BP:78:PRO:C     | 37:BP:79:VAL:HG23  | 2.45                     | 0.41              |
| 40:BS:6:LYS:CB     | 40:BS:104:THR:HG22 | 2.50                     | 0.41              |
| 42:BU:60:LYS:CG    | 42:BU:61:GLU:N     | 2.84                     | 0.41              |
| 42:BU:82:VAL:HG12  | 42:BU:83:GLY:N     | 2.35                     | 0.41              |
| 42:BU:92:VAL:O     | 42:BU:93:ARG:C     | 2.64                     | 0.41              |
| 43:BW:54:ARG:HH11  | 43:BW:54:ARG:CG    | 2.31                     | 0.41              |
| 46:BZ:21:VAL:HG12  | 46:BZ:23:LYS:HG2   | 2.03                     | 0.41              |
| 1:CA:191:G:H2'     | 1:CA:192:A:C8      | 2.56                     | 0.41              |
| 1:CA:652:U:O4      | 1:CA:752:G:O2'     | 2.37                     | 0.41              |
| 1:CA:844:G:H2'     | 1:CA:845:A:H5''    | 2.01                     | 0.41              |
| 1:CA:1043:G:C2'    | 1:CA:1044:A:O5'    | 2.68                     | 0.41              |
| 1:CA:1128:C:H2'    | 1:CA:1129:C:O4'    | 2.21                     | 0.41              |
| 1:CA:1170:A:H5''   | 20:CB:138:ARG:HH22 | 1.84                     | 0.41              |
| 1:CA:1294:G:H2'    | 1:CA:1295:U:C6     | 2.56                     | 0.41              |
| 1:CA:1510:C:H2'    | 1:CA:1511:G:C8     | 2.56                     | 0.41              |
| 3:CD:115:GLN:HE21  | 3:CD:153:ARG:HH12  | 1.66                     | 0.41              |
| 6:CG:70:PRO:HD3    | 6:CG:102:TRP:CZ3   | 2.56                     | 0.41              |
| 8:CI:10:ARG:HA     | 8:CI:14:SER:O      | 2.21                     | 0.41              |
| 8:CI:30:ASN:CG     | 8:CI:65:THR:HA     | 2.46                     | 0.41              |
| 9:CJ:92:LEU:O      | 9:CJ:93:ALA:HB2    | 2.21                     | 0.41              |
| 12:CM:13:HIS:HB2   | 12:CM:16:ILE:HG22  | 2.02                     | 0.41              |
| 13:CN:12:ARG:HD3   | 13:CN:58:ARG:O     | 2.20                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:CQ:64:ARG:HH11  | 16:CQ:64:ARG:CB    | 2.34                     | 0.41              |
| 18:CS:28:LYS:HB2   | 18:CS:29:PRO:HD2   | 2.02                     | 0.41              |
| 19:CT:24:ARG:HG3   | 19:CT:65:LEU:HD11  | 2.03                     | 0.41              |
| 23:DB:31:C:C2'     | 23:DB:32:C:H5'     | 2.51                     | 0.41              |
| 23:DB:67:U:H2'     | 23:DB:68:G:O4'     | 2.21                     | 0.41              |
| 23:DB:484:C:H2'    | 23:DB:485:C:C6     | 2.54                     | 0.41              |
| 23:DB:622:G:H2'    | 23:DB:623:C:H6     | 1.86                     | 0.41              |
| 23:DB:1322:A:C5    | 23:DB:1323:C:C5    | 3.08                     | 0.41              |
| 23:DB:1446:C:H2'   | 23:DB:1447:C:H6    | 1.86                     | 0.41              |
| 23:DB:1498:C:H2'   | 23:DB:1499:C:H6    | 1.86                     | 0.41              |
| 23:DB:1744:A:O2'   | 23:DB:1745:A:H5'   | 2.21                     | 0.41              |
| 23:DB:2070:A:C2    | 23:DB:2442:C:C2    | 3.09                     | 0.41              |
| 23:DB:2259:U:C2    | 23:DB:2260:C:C6    | 3.09                     | 0.41              |
| 25:DC:265:PHE:HB3  | 25:DC:266:ILE:H    | 1.75                     | 0.41              |
| 26:DD:61:THR:O     | 26:DD:62:LYS:C     | 2.64                     | 0.41              |
| 28:DF:35:LEU:CD2   | 28:DF:153:ILE:HG12 | 2.51                     | 0.41              |
| 29:DG:2:ARG:O      | 29:DG:2:ARG:HD2    | 2.21                     | 0.41              |
| 29:DG:121:THR:HG22 | 29:DG:122:ALA:H    | 1.86                     | 0.41              |
| 29:DG:145:ALA:HB2  | 29:DG:163:TYR:OH   | 2.20                     | 0.41              |
| 29:DG:156:TYR:HD1  | 29:DG:171:LYS:HG2  | 1.85                     | 0.41              |
| 30:DH:3:VAL:CB     | 30:DH:37:VAL:HG11  | 2.50                     | 0.41              |
| 33:DL:59:ARG:C     | 50:D3:11:LYS:HE2   | 2.45                     | 0.41              |
| 33:DL:66:PHE:CD2   | 33:DL:67:THR:N     | 2.89                     | 0.41              |
| 35:DN:14:SER:HA    | 35:DN:17:ARG:CZ    | 2.51                     | 0.41              |
| 37:DP:91:VAL:O     | 37:DP:92:ARG:HB3   | 2.21                     | 0.41              |
| 39:DR:20:VAL:HA    | 39:DR:97:LYS:O     | 2.20                     | 0.41              |
| 39:DR:35:PHE:O     | 39:DR:63:VAL:HG23  | 2.20                     | 0.41              |
| 41:DT:61:LEU:O     | 41:DT:62:VAL:HG13  | 2.21                     | 0.41              |
| 45:DY:58:GLU:CD    | 45:DY:58:GLU:H     | 2.29                     | 0.41              |
| 48:D1:8:ILE:HG23   | 48:D1:9:LYS:N      | 2.35                     | 0.41              |
| 50:D3:38:LYS:N     | 50:D3:38:LYS:HD2   | 2.36                     | 0.41              |
| 52:DI:131:THR:O    | 52:DI:135:MET:HG3  | 2.21                     | 0.41              |
| 1:AA:31:G:H2'      | 1:AA:48:C:H41      | 1.86                     | 0.41              |
| 1:AA:91:U:H2'      | 1:AA:92:U:C6       | 2.56                     | 0.41              |
| 1:AA:144:G:H2'     | 1:AA:145:G:C8      | 2.56                     | 0.41              |
| 1:AA:208:U:H2'     | 1:AA:210:C:C6      | 2.55                     | 0.41              |
| 1:AA:401:C:H2'     | 1:AA:402:G:H8      | 1.86                     | 0.41              |
| 1:AA:493:A:N3      | 1:AA:493:A:O4'     | 2.54                     | 0.41              |
| 1:AA:601:G:O2'     | 1:AA:602:A:H5'     | 2.21                     | 0.41              |
| 1:AA:688:G:O2'     | 1:AA:689:C:H5'     | 2.20                     | 0.41              |
| 1:AA:737:C:H2'     | 1:AA:738:C:C6      | 2.55                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:846:G:H5'    | 1:AA:847:G:OP2    | 2.21                     | 0.41              |
| 1:AA:890:G:O2'    | 1:AA:906:A:N6     | 2.53                     | 0.41              |
| 1:AA:955:U:H2'    | 1:AA:956:U:O4'    | 2.21                     | 0.41              |
| 1:AA:960:U:C1'    | 1:AA:961:U:OP2    | 2.69                     | 0.41              |
| 1:AA:1005:A:C2'   | 1:AA:1006:G:H5'   | 2.51                     | 0.41              |
| 1:AA:1033:G:C3'   | 1:AA:1034:G:H5''  | 2.51                     | 0.41              |
| 1:AA:1057:G:H4'   | 2:AC:194:VAL:O    | 2.21                     | 0.41              |
| 1:AA:1148:U:C2'   | 1:AA:1149:C:H5'   | 2.50                     | 0.41              |
| 1:AA:1245:C:O2'   | 1:AA:1246:A:H5'   | 2.20                     | 0.41              |
| 1:AA:1258:G:O2'   | 1:AA:1259:C:H5'   | 2.21                     | 0.41              |
| 1:AA:1458:G:H2'   | 1:AA:1459:G:C8    | 2.56                     | 0.41              |
| 1:AA:1523:G:H2'   | 1:AA:1524:C:C6    | 2.55                     | 0.41              |
| 2:AC:137:VAL:HG11 | 2:AC:150:VAL:HG21 | 2.01                     | 0.41              |
| 2:AC:139:ASN:N    | 2:AC:139:ASN:ND2  | 2.68                     | 0.41              |
| 2:AC:176:THR:O    | 2:AC:179:ALA:HB3  | 2.21                     | 0.41              |
| 2:AC:178:ARG:O    | 2:AC:206:ILE:HA   | 2.21                     | 0.41              |
| 3:AD:37:PRO:HD2   | 3:AD:41:GLY:CA    | 2.51                     | 0.41              |
| 3:AD:55:ARG:NH2   | 3:AD:58:GLN:NE2   | 2.67                     | 0.41              |
| 3:AD:89:LEU:O     | 3:AD:92:LEU:HB2   | 2.21                     | 0.41              |
| 3:AD:138:PRO:C    | 3:AD:140:ASP:H    | 2.29                     | 0.41              |
| 5:AF:7:VAL:HB     | 5:AF:61:LEU:HD22  | 2.03                     | 0.41              |
| 5:AF:38:ARG:HH21  | 5:AF:96:VAL:CG1   | 2.33                     | 0.41              |
| 6:AG:94:ARG:NH1   | 6:AG:98:LEU:HD11  | 2.35                     | 0.41              |
| 7:AH:9:MET:O      | 7:AH:13:ILE:HG13  | 2.20                     | 0.41              |
| 8:AI:35:GLU:N     | 8:AI:35:GLU:OE2   | 2.54                     | 0.41              |
| 8:AI:56:MET:HA    | 8:AI:59:LYS:HB2   | 2.03                     | 0.41              |
| 9:AJ:67:ILE:CG1   | 13:AN:95:LEU:HD13 | 2.44                     | 0.41              |
| 10:AK:122:PRO:HG2 | 21:AU:35:GLU:HG2  | 2.02                     | 0.41              |
| 12:AM:94:LEU:HD22 | 12:AM:101:THR:OG1 | 2.21                     | 0.41              |
| 14:AO:15:GLY:HA3  | 14:AO:20:ASP:OD1  | 2.21                     | 0.41              |
| 14:AO:52:ARG:HG3  | 14:AO:55:LEU:HD23 | 2.03                     | 0.41              |
| 14:AO:71:ARG:NH1  | 14:AO:71:ARG:HB2  | 2.35                     | 0.41              |
| 16:AQ:8:GLN:HA    | 16:AQ:58:VAL:O    | 2.21                     | 0.41              |
| 17:AR:24:ASP:O    | 17:AR:28:LEU:HD13 | 2.20                     | 0.41              |
| 17:AR:32:ILE:HG13 | 17:AR:33:THR:N    | 2.35                     | 0.41              |
| 19:AT:20:ASN:HA   | 19:AT:65:LEU:HD21 | 2.02                     | 0.41              |
| 19:AT:57:VAL:C    | 19:AT:60:GLN:NE2  | 2.78                     | 0.41              |
| 20:AB:85:SER:C    | 20:AB:87:ASP:H    | 2.29                     | 0.41              |
| 20:AB:96:LEU:HD23 | 20:AB:99:MET:CE   | 2.50                     | 0.41              |
| 20:AB:114:LYS:HA  | 20:AB:117:GLU:OE1 | 2.21                     | 0.41              |
| 20:AB:202:ASN:ND2 | 20:AB:204:ASP:N   | 2.60                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:BA:86:G:H3'     | 22:BA:87:U:H6      | 1.84                     | 0.41              |
| 22:BA:95:U:H2'     | 22:BA:96:G:C8      | 2.55                     | 0.41              |
| 23:BB:134:G:C6     | 23:BB:146:A:C6     | 3.08                     | 0.41              |
| 23:BB:137:U:H2'    | 23:BB:138:U:C5'    | 2.51                     | 0.41              |
| 23:BB:196:A:N7     | 33:BL:52:GLY:HA2   | 2.36                     | 0.41              |
| 23:BB:286:U:H2'    | 23:BB:287:G:H8     | 1.86                     | 0.41              |
| 23:BB:356:G:O2'    | 23:BB:357:C:H5'    | 2.20                     | 0.41              |
| 23:BB:503:A:H5''   | 23:BB:504:A:H5'    | 2.02                     | 0.41              |
| 23:BB:607:U:C4     | 23:BB:620:G:O4'    | 2.73                     | 0.41              |
| 23:BB:723:C:H2'    | 23:BB:724:U:H6     | 1.84                     | 0.41              |
| 23:BB:794:A:C4     | 23:BB:795:C:C5     | 3.09                     | 0.41              |
| 23:BB:849:A:H2'    | 23:BB:850:U:C6     | 2.55                     | 0.41              |
| 23:BB:1142:A:C4    | 23:BB:1144:A:C8    | 3.08                     | 0.41              |
| 23:BB:1192:G:C2'   | 23:BB:1193:G:H5'   | 2.50                     | 0.41              |
| 23:BB:1225:G:C5'   | 39:BR:78:ARG:NH2   | 2.84                     | 0.41              |
| 23:BB:1460:U:H5''  | 23:BB:1461:C:C6    | 2.56                     | 0.41              |
| 23:BB:1568:G:H5''  | 25:BC:60:ALA:HB3   | 2.02                     | 0.41              |
| 23:BB:1764:C:H2'   | 23:BB:1765:U:C6    | 2.56                     | 0.41              |
| 23:BB:1795:C:H2'   | 23:BB:1796:U:H6    | 1.85                     | 0.41              |
| 23:BB:1989:G:H2'   | 23:BB:1990:C:O4'   | 2.21                     | 0.41              |
| 23:BB:2019:A:O2'   | 38:BQ:32:ARG:NH2   | 2.54                     | 0.41              |
| 23:BB:2020:A:OP1   | 38:BQ:25:GLY:HA3   | 2.20                     | 0.41              |
| 23:BB:2026:U:H2'   | 23:BB:2027:G:C8    | 2.55                     | 0.41              |
| 23:BB:2441:U:O2'   | 23:BB:2442:C:H5'   | 2.21                     | 0.41              |
| 23:BB:2545:G:N3    | 23:BB:2565:A:H2    | 2.19                     | 0.41              |
| 23:BB:2617:U:O2'   | 23:BB:2618:G:H5'   | 2.21                     | 0.41              |
| 23:BB:2720:U:H2'   | 23:BB:2721:A:C8    | 2.55                     | 0.41              |
| 23:BB:2897:U:H2'   | 23:BB:2898:U:C6    | 2.55                     | 0.41              |
| 24:BV:87:GLN:NE2   | 24:BV:87:GLN:N     | 2.69                     | 0.41              |
| 25:BC:24:HIS:HB3   | 25:BC:27:LYS:HE3   | 2.03                     | 0.41              |
| 25:BC:37:SER:H     | 25:BC:62:ARG:HB2   | 1.86                     | 0.41              |
| 25:BC:107:LYS:H    | 25:BC:194:VAL:CG2  | 2.31                     | 0.41              |
| 25:BC:143:VAL:HG12 | 25:BC:187:CYS:SG   | 2.61                     | 0.41              |
| 25:BC:160:TYR:CD2  | 25:BC:193:GLU:HG2  | 2.56                     | 0.41              |
| 26:BD:46:ARG:HD2   | 26:BD:80:TRP:CH2   | 2.55                     | 0.41              |
| 26:BD:140:HIS:O    | 26:BD:142:VAL:N    | 2.54                     | 0.41              |
| 26:BD:170:VAL:CG1  | 26:BD:194:PRO:HG2  | 2.51                     | 0.41              |
| 27:BE:25:GLU:O     | 27:BE:27:LEU:N     | 2.54                     | 0.41              |
| 27:BE:83:VAL:O     | 27:BE:84:THR:C     | 2.64                     | 0.41              |
| 27:BE:146:VAL:HG23 | 27:BE:148:ILE:HG23 | 2.02                     | 0.41              |
| 27:BE:153:LEU:HD11 | 27:BE:193:VAL:HG11 | 2.02                     | 0.41              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BE:190:ALA:HB1  | 27:BE:193:VAL:CB   | 2.50                     | 0.41              |
| 30:BH:41:LYS:HD2   | 30:BH:41:LYS:N     | 2.33                     | 0.41              |
| 30:BH:66:ASN:OD1   | 30:BH:138:VAL:HG11 | 2.20                     | 0.41              |
| 30:BH:69:ALA:HB1   | 30:BH:141:LYS:HZ3  | 1.85                     | 0.41              |
| 31:BJ:84:ILE:CG2   | 31:BJ:85:LYS:H     | 2.31                     | 0.41              |
| 31:BJ:125:TYR:CE2  | 31:BJ:134:ALA:HB2  | 2.56                     | 0.41              |
| 32:BK:108:ARG:HG3  | 32:BK:108:ARG:NH1  | 2.36                     | 0.41              |
| 33:BL:81:ASP:O     | 33:BL:82:LEU:C     | 2.63                     | 0.41              |
| 33:BL:84:LYS:O     | 33:BL:85:VAL:CB    | 2.69                     | 0.41              |
| 33:BL:88:GLY:C     | 33:BL:90:VAL:N     | 2.79                     | 0.41              |
| 33:BL:118:THR:OG1  | 33:BL:119:PRO:HD3  | 2.20                     | 0.41              |
| 33:BL:125:LEU:C    | 33:BL:126:ARG:HG3  | 2.46                     | 0.41              |
| 34:BM:8:LYS:NZ     | 34:BM:69:PRO:HG2   | 2.36                     | 0.41              |
| 34:BM:45:GLN:CG    | 34:BM:120:ALA:HA   | 2.51                     | 0.41              |
| 36:BO:105:ALA:HA   | 36:BO:108:ASP:OD2  | 2.21                     | 0.41              |
| 36:BO:114:GLY:O    | 36:BO:115:LEU:C    | 2.63                     | 0.41              |
| 37:BP:45:VAL:HG12  | 37:BP:65:ASN:HB2   | 2.02                     | 0.41              |
| 37:BP:59:THR:O     | 37:BP:59:THR:HG22  | 2.20                     | 0.41              |
| 38:BQ:4:LYS:C      | 38:BQ:6:GLY:N      | 2.79                     | 0.41              |
| 38:BQ:35:PHE:HE1   | 39:BR:85:LYS:NZ    | 2.19                     | 0.41              |
| 38:BQ:108:LEU:HD21 | 39:BR:52:PRO:O     | 2.21                     | 0.41              |
| 41:BT:33:LYS:O     | 41:BT:34:VAL:C     | 2.64                     | 0.41              |
| 42:BU:9:GLU:CG     | 42:BU:23:LYS:HB3   | 2.51                     | 0.41              |
| 42:BU:71:ILE:HG21  | 42:BU:95:PHE:CE1   | 2.55                     | 0.41              |
| 43:BW:81:ILE:HG13  | 43:BW:82:GLU:HG2   | 2.03                     | 0.41              |
| 45:BY:16:LEU:CB    | 45:BY:17:PRO:CD    | 2.91                     | 0.41              |
| 46:BZ:3:LYS:HG3    | 46:BZ:6:HIS:O      | 2.21                     | 0.41              |
| 48:B1:29:LYS:CE    | 48:B1:30:PRO:HD2   | 2.47                     | 0.41              |
| 49:B2:9:VAL:O      | 49:B2:12:ARG:HB2   | 2.20                     | 0.41              |
| 50:B3:19:GLY:O     | 50:B3:20:GLY:C     | 2.62                     | 0.41              |
| 51:B4:11:CYS:SG    | 51:B4:12:ARG:N     | 2.94                     | 0.41              |
| 51:B4:24:ARG:NH2   | 51:B4:36:ARG:HH11  | 2.19                     | 0.41              |
| 52:BI:16:MET:N     | 52:BI:42:ASN:OD1   | 2.54                     | 0.41              |
| 1:CA:90:C:H2'      | 1:CA:91:U:H6       | 1.84                     | 0.41              |
| 1:CA:181:A:H1'     | 1:CA:182:A:C2      | 2.56                     | 0.41              |
| 1:CA:359:G:O2'     | 1:CA:360:G:H5'     | 2.21                     | 0.41              |
| 1:CA:407:U:O2'     | 3:CD:112:GLU:HG3   | 2.21                     | 0.41              |
| 1:CA:599:C:H2'     | 1:CA:600:A:H8      | 1.85                     | 0.41              |
| 1:CA:607:A:H2'     | 1:CA:608:A:H8      | 1.86                     | 0.41              |
| 1:CA:672:U:H2'     | 1:CA:673:A:H8      | 1.83                     | 0.41              |
| 1:CA:728:A:H2'     | 1:CA:729:A:C8      | 2.55                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:737:C:H2'    | 1:CA:738:C:C6     | 2.55                     | 0.41              |
| 1:CA:738:C:H2'    | 1:CA:739:C:H6     | 1.86                     | 0.41              |
| 1:CA:746:A:H2'    | 1:CA:747:A:H8     | 1.86                     | 0.41              |
| 1:CA:750:C:O2     | 14:CO:22:GLY:HA3  | 2.21                     | 0.41              |
| 1:CA:828:U:H2'    | 1:CA:829:G:O5'    | 2.21                     | 0.41              |
| 1:CA:830:G:H2'    | 1:CA:831:A:H8     | 1.86                     | 0.41              |
| 1:CA:982:U:OP2    | 13:CN:5:MET:HE1   | 2.21                     | 0.41              |
| 1:CA:984:C:H2'    | 1:CA:985:C:C6     | 2.56                     | 0.41              |
| 1:CA:1039:G:O2'   | 1:CA:1040:U:H5'   | 2.21                     | 0.41              |
| 1:CA:1317:C:H42   | 18:CS:36:ARG:NH2  | 2.18                     | 0.41              |
| 3:CD:147:LYS:HD3  | 3:CD:147:LYS:C    | 2.46                     | 0.41              |
| 3:CD:190:LEU:O    | 3:CD:191:SER:C    | 2.63                     | 0.41              |
| 4:CE:95:MET:CE    | 4:CE:143:LEU:HD13 | 2.43                     | 0.41              |
| 4:CE:109:ALA:HB1  | 4:CE:136:VAL:CG1  | 2.49                     | 0.41              |
| 7:CH:100:ILE:HD12 | 7:CH:101:ALA:N    | 2.36                     | 0.41              |
| 8:CI:20:ILE:CG2   | 8:CI:60:LEU:HD22  | 2.51                     | 0.41              |
| 8:CI:107:ALA:O    | 8:CI:108:ARG:C    | 2.64                     | 0.41              |
| 8:CI:109:GLN:HE21 | 8:CI:109:GLN:HB3  | 1.61                     | 0.41              |
| 11:CL:29:LYS:HB3  | 11:CL:56:LEU:HD22 | 2.02                     | 0.41              |
| 11:CL:49:ARG:CD   | 11:CL:89:LEU:HD21 | 2.51                     | 0.41              |
| 12:CM:102:LYS:HB2 | 12:CM:102:LYS:HZ2 | 1.82                     | 0.41              |
| 14:CO:49:HIS:O    | 14:CO:52:ARG:HB3  | 2.21                     | 0.41              |
| 16:CQ:57:VAL:HB   | 16:CQ:79:GLU:HB2  | 2.03                     | 0.41              |
| 18:CS:41:PRO:HA   | 18:CS:44:ILE:CG1  | 2.50                     | 0.41              |
| 19:CT:5:SER:C     | 19:CT:7:LYS:H     | 2.29                     | 0.41              |
| 20:CB:94:ARG:O    | 20:CB:95:TRP:C    | 2.63                     | 0.41              |
| 21:CU:35:GLU:HA   | 21:CU:35:GLU:OE1  | 2.20                     | 0.41              |
| 22:DA:92:C:H2'    | 22:DA:93:C:C6     | 2.56                     | 0.41              |
| 23:DB:103:A:H3'   | 23:DB:104:A:H8    | 1.85                     | 0.41              |
| 23:DB:247:G:O6    | 50:D3:7:ARG:HD2   | 2.21                     | 0.41              |
| 23:DB:296:U:H3'   | 55:DB:3414:HOH:O  | 2.21                     | 0.41              |
| 23:DB:301:G:C4    | 23:DB:302:C:C6    | 3.09                     | 0.41              |
| 23:DB:443:A:C8    | 27:DE:40:ARG:HG2  | 2.55                     | 0.41              |
| 23:DB:583:G:H2'   | 23:DB:584:C:H6    | 1.86                     | 0.41              |
| 23:DB:619:G:H3'   | 23:DB:620:G:H21   | 1.86                     | 0.41              |
| 23:DB:820:A:H2'   | 23:DB:821:A:O4'   | 2.20                     | 0.41              |
| 23:DB:869:G:H2'   | 23:DB:870:U:O4'   | 2.20                     | 0.41              |
| 23:DB:1099:G:C5'  | 52:DI:3:LYS:CA    | 2.99                     | 0.41              |
| 23:DB:1120:G:H2'  | 23:DB:1121:C:C6   | 2.56                     | 0.41              |
| 23:DB:1268:A:H2'  | 23:DB:1269:A:C8   | 2.55                     | 0.41              |
| 23:DB:1390:U:O2'  | 23:DB:1391:U:H5'  | 2.20                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:1528:A:C2'   | 23:DB:1529:G:H5'   | 2.50                     | 0.41              |
| 23:DB:1593:A:H2'   | 23:DB:1594:U:O4'   | 2.20                     | 0.41              |
| 23:DB:1655:A:H2'   | 23:DB:1656:C:O4'   | 2.21                     | 0.41              |
| 23:DB:1825:U:H5'   | 25:DC:244:VAL:HG23 | 1.99                     | 0.41              |
| 23:DB:1841:U:H2'   | 23:DB:1842:G:C8    | 2.55                     | 0.41              |
| 23:DB:1897:G:O2'   | 23:DB:1898:U:H5'   | 2.20                     | 0.41              |
| 23:DB:1924:C:O2'   | 23:DB:1925:C:H5'   | 2.21                     | 0.41              |
| 23:DB:2045:C:H5''  | 47:D0:14:MET:HE3   | 2.03                     | 0.41              |
| 23:DB:2188:U:O2'   | 23:DB:2189:U:H5'   | 2.21                     | 0.41              |
| 23:DB:2559:C:O2'   | 23:DB:2560:A:H5'   | 2.19                     | 0.41              |
| 23:DB:2597:G:OP1   | 25:DC:239:PHE:CD2  | 2.74                     | 0.41              |
| 23:DB:2665:A:H2'   | 23:DB:2666:C:O2    | 2.21                     | 0.41              |
| 23:DB:2710:C:H2'   | 23:DB:2711:A:C8    | 2.56                     | 0.41              |
| 24:DV:43:ASP:O     | 24:DV:47:VAL:HG23  | 2.20                     | 0.41              |
| 25:DC:103:ILE:HG22 | 25:DC:104:LEU:N    | 2.36                     | 0.41              |
| 25:DC:163:ILE:HA   | 25:DC:173:LEU:HD23 | 2.03                     | 0.41              |
| 25:DC:173:LEU:HD12 | 25:DC:183:VAL:CG1  | 2.48                     | 0.41              |
| 26:DD:26:VAL:O     | 26:DD:26:VAL:HG13  | 2.21                     | 0.41              |
| 26:DD:151:THR:C    | 26:DD:153:GLY:N    | 2.79                     | 0.41              |
| 26:DD:197:THR:CG2  | 26:DD:198:GLY:H    | 2.08                     | 0.41              |
| 27:DE:10:SER:C     | 27:DE:12:LEU:N     | 2.78                     | 0.41              |
| 27:DE:48:THR:CG2   | 27:DE:85:PHE:N     | 2.84                     | 0.41              |
| 28:DF:98:PHE:HA    | 28:DF:101:ARG:CG   | 2.50                     | 0.41              |
| 28:DF:99:PHE:CD1   | 28:DF:102:LEU:HD23 | 2.56                     | 0.41              |
| 29:DG:152:ARG:HA   | 29:DG:153:PRO:HD3  | 1.96                     | 0.41              |
| 31:DJ:21:THR:HG22  | 31:DJ:58:ASN:CG    | 2.46                     | 0.41              |
| 31:DJ:36:LEU:O     | 31:DJ:51:GLY:HA2   | 2.21                     | 0.41              |
| 31:DJ:128:ASN:O    | 31:DJ:130:HIS:N    | 2.54                     | 0.41              |
| 33:DL:33:ARG:HB3   | 39:DR:85:LYS:NZ    | 2.35                     | 0.41              |
| 35:DN:106:ASP:O    | 35:DN:107:ASN:HB3  | 2.20                     | 0.41              |
| 36:DO:10:ARG:HD2   | 36:DO:94:ARG:HG3   | 2.02                     | 0.41              |
| 36:DO:30:ARG:CD    | 36:DO:97:PHE:HD2   | 2.33                     | 0.41              |
| 37:DP:61:ARG:CZ    | 37:DP:61:ARG:CB    | 2.98                     | 0.41              |
| 37:DP:91:VAL:O     | 37:DP:92:ARG:CB    | 2.69                     | 0.41              |
| 37:DP:109:ILE:O    | 37:DP:110:LYS:C    | 2.64                     | 0.41              |
| 38:DQ:68:ALA:C     | 38:DQ:73:ILE:HG21  | 2.46                     | 0.41              |
| 40:DS:20:VAL:O     | 40:DS:24:ILE:HG13  | 2.21                     | 0.41              |
| 42:DU:26:ASN:O     | 42:DU:28:LEU:HG    | 2.21                     | 0.41              |
| 42:DU:27:VAL:C     | 42:DU:28:LEU:HG    | 2.45                     | 0.41              |
| 42:DU:71:ILE:CG1   | 42:DU:72:PHE:N     | 2.84                     | 0.41              |
| 43:DW:18:LYS:HG3   | 43:DW:19:ARG:N     | 2.36                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 43:DW:75:ASN:C     | 43:DW:77:LYS:N    | 2.78                     | 0.41              |
| 44:DX:19:LEU:C     | 44:DX:21:LEU:N    | 2.79                     | 0.41              |
| 44:DX:40:SER:OG    | 44:DX:42:LEU:HD23 | 2.20                     | 0.41              |
| 44:DX:41:HIS:ND1   | 44:DX:43:LEU:HD23 | 2.36                     | 0.41              |
| 45:DY:5:LYS:NZ     | 45:DY:5:LYS:CB    | 2.84                     | 0.41              |
| 46:DZ:1:MET:HG3    | 46:DZ:9:TYR:CE2   | 2.56                     | 0.41              |
| 46:DZ:11:GLU:O     | 46:DZ:27:THR:HG22 | 2.21                     | 0.41              |
| 46:DZ:20:ASN:O     | 46:DZ:21:VAL:CB   | 2.63                     | 0.41              |
| 48:D1:5:ARG:NH1    | 48:D1:5:ARG:HG2   | 2.35                     | 0.41              |
| 48:D1:34:GLU:HB3   | 48:D1:50:GLU:HB3  | 2.03                     | 0.41              |
| 50:D3:32:LEU:HD22  | 50:D3:32:LEU:HA   | 1.93                     | 0.41              |
| 51:D4:16:ILE:C     | 51:D4:18:LYS:N    | 2.78                     | 0.41              |
| 51:D4:23:ILE:CD1   | 51:D4:24:ARG:HH11 | 2.34                     | 0.41              |
| 51:D4:36:ARG:HG2   | 51:D4:36:ARG:NH1  | 2.34                     | 0.41              |
| 52:DI:100:ILE:CG2  | 52:DI:104:GLN:HB2 | 2.50                     | 0.41              |
| 1:AA:358:U:H2'     | 1:AA:359:G:H8     | 1.86                     | 0.41              |
| 1:AA:359:G:O2'     | 1:AA:360:G:H5'    | 2.21                     | 0.41              |
| 1:AA:367:U:OP1     | 1:AA:395:C:H1'    | 2.21                     | 0.41              |
| 1:AA:393:A:O2'     | 1:AA:394:G:H5'    | 2.20                     | 0.41              |
| 1:AA:580:C:H2'     | 1:AA:581:G:O4'    | 2.21                     | 0.41              |
| 1:AA:611:C:H2'     | 1:AA:612:C:C6     | 2.56                     | 0.41              |
| 1:AA:612:C:H2'     | 1:AA:613:C:C6     | 2.56                     | 0.41              |
| 1:AA:1276:G:H2'    | 1:AA:1277:C:C6    | 2.56                     | 0.41              |
| 1:AA:1401:G:O2'    | 1:AA:1402:C:H5'   | 2.20                     | 0.41              |
| 3:AD:170:LEU:HD12  | 3:AD:170:LEU:C    | 2.46                     | 0.41              |
| 3:AD:197:HIS:HA    | 3:AD:200:VAL:HG22 | 2.03                     | 0.41              |
| 4:AE:81:GLN:NE2    | 4:AE:82:HIS:ND1   | 2.68                     | 0.41              |
| 8:AI:9:GLY:O       | 8:AI:16:ALA:HB3   | 2.21                     | 0.41              |
| 8:AI:52:GLU:N      | 8:AI:56:MET:HG2   | 2.35                     | 0.41              |
| 13:AN:68:ARG:HH11  | 13:AN:70:HIS:HB2  | 1.85                     | 0.41              |
| 16:AQ:10:ARG:HD3   | 16:AQ:55:GLY:H    | 1.86                     | 0.41              |
| 20:AB:140:LEU:HD22 | 20:AB:144:GLU:OE2 | 2.20                     | 0.41              |
| 21:AU:38:GLU:C     | 21:AU:38:GLU:CD   | 2.88                     | 0.41              |
| 22:BA:109:A:O2'    | 22:BA:110:C:H5'   | 2.20                     | 0.41              |
| 23:BB:28:A:H2'     | 23:BB:29:U:H6     | 1.85                     | 0.41              |
| 23:BB:197:A:H4'    | 23:BB:2069:G:OP2  | 2.21                     | 0.41              |
| 23:BB:264:C:C2'    | 23:BB:265:A:H5''  | 2.51                     | 0.41              |
| 23:BB:527:C:H5''   | 23:BB:2779:U:N3   | 2.36                     | 0.41              |
| 23:BB:570:G:C2'    | 23:BB:571:U:H5'   | 2.51                     | 0.41              |
| 23:BB:730:A:C2     | 23:BB:731:C:C6    | 3.09                     | 0.41              |
| 23:BB:820:A:H2'    | 23:BB:821:A:O4'   | 2.21                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:1060:U:C1'  | 23:BB:1062:G:H5'   | 2.51                     | 0.41              |
| 23:BB:1170:C:O2'  | 23:BB:1171:G:H5'   | 2.21                     | 0.41              |
| 23:BB:1198:U:H2'  | 23:BB:1199:U:C5    | 2.55                     | 0.41              |
| 23:BB:1449:G:H2'  | 23:BB:1450:G:C8    | 2.56                     | 0.41              |
| 23:BB:1936:A:C2   | 23:BB:1943:U:H5    | 2.39                     | 0.41              |
| 23:BB:2139:U:O5'  | 23:BB:2139:U:H6    | 2.04                     | 0.41              |
| 23:BB:2621:G:P    | 26:BD:124:ARG:HH22 | 2.44                     | 0.41              |
| 23:BB:2693:G:O2'  | 23:BB:2694:G:H5'   | 2.21                     | 0.41              |
| 24:BV:76:ASP:HB2  | 34:BM:136:MET:CE   | 2.49                     | 0.41              |
| 25:BC:152:GLN:HB3 | 25:BC:153:LEU:H    | 1.53                     | 0.41              |
| 25:BC:205:GLY:O   | 25:BC:206:LYS:HG2  | 2.21                     | 0.41              |
| 28:BF:116:LEU:HG  | 28:BF:175:PRO:O    | 2.21                     | 0.41              |
| 31:BJ:7:LYS:HZ3   | 31:BJ:48:VAL:CA    | 2.34                     | 0.41              |
| 31:BJ:16:TYR:HD2  | 31:BJ:140:LEU:HB2  | 1.86                     | 0.41              |
| 32:BK:69:VAL:C    | 32:BK:76:VAL:HG13  | 2.46                     | 0.41              |
| 33:BL:2:ARG:NH1   | 33:BL:4:ASN:HD21   | 2.19                     | 0.41              |
| 34:BM:8:LYS:HZ2   | 34:BM:69:PRO:HB2   | 1.84                     | 0.41              |
| 34:BM:8:LYS:NZ    | 34:BM:69:PRO:HB2   | 2.36                     | 0.41              |
| 35:BN:103:ARG:HG2 | 35:BN:103:ARG:O    | 2.21                     | 0.41              |
| 36:BO:36:TYR:HA   | 36:BO:52:SER:HB2   | 2.03                     | 0.41              |
| 37:BP:28:LYS:HB3  | 37:BP:44:GLY:H     | 1.85                     | 0.41              |
| 38:BQ:50:ARG:HH11 | 38:BQ:50:ARG:HG2   | 1.86                     | 0.41              |
| 39:BR:73:LYS:O    | 39:BR:74:ILE:O     | 2.39                     | 0.41              |
| 40:BS:37:THR:HG23 | 40:BS:38:TYR:CD1   | 2.56                     | 0.41              |
| 42:BU:38:ILE:HB   | 42:BU:62:ALA:HB3   | 2.03                     | 0.41              |
| 42:BU:41:VAL:HG13 | 42:BU:41:VAL:O     | 2.20                     | 0.41              |
| 43:BW:14:ASP:O    | 43:BW:15:SER:HB3   | 2.21                     | 0.41              |
| 44:BX:50:VAL:O    | 44:BX:53:VAL:HG23  | 2.21                     | 0.41              |
| 45:BY:31:ILE:C    | 45:BY:33:HIS:H     | 2.28                     | 0.41              |
| 48:B1:11:VAL:HG13 | 48:B1:12:SER:N     | 2.35                     | 0.41              |
| 49:B2:10:LEU:HD23 | 49:B2:10:LEU:C     | 2.46                     | 0.41              |
| 49:B2:39:ARG:NH1  | 49:B2:39:ARG:HB2   | 2.35                     | 0.41              |
| 1:CA:175:C:H2'    | 1:CA:176:C:H6      | 1.86                     | 0.41              |
| 1:CA:208:U:C2'    | 1:CA:209:U:H5''    | 2.50                     | 0.41              |
| 1:CA:276:G:O2'    | 1:CA:277:C:H5'     | 2.21                     | 0.41              |
| 1:CA:358:U:H2'    | 1:CA:359:G:H8      | 1.86                     | 0.41              |
| 1:CA:493:A:N3     | 1:CA:493:A:O4'     | 2.54                     | 0.41              |
| 1:CA:691:G:H1'    | 1:CA:696:A:H61     | 1.84                     | 0.41              |
| 1:CA:878:A:H2'    | 1:CA:879:C:C6      | 2.56                     | 0.41              |
| 1:CA:1004:A:H3'   | 1:CA:1005:A:C8     | 2.54                     | 0.41              |
| 1:CA:1015:G:O2'   | 1:CA:1016:A:H5'    | 2.21                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1018:G:H2'   | 1:CA:1019:A:C8    | 2.55                     | 0.41              |
| 1:CA:1029:U:N3    | 1:CA:1033:G:C2    | 2.89                     | 0.41              |
| 2:CC:37:LYS:HB3   | 2:CC:41:TYR:CE1   | 2.56                     | 0.41              |
| 2:CC:91:ALA:HB2   | 2:CC:98:ALA:CB    | 2.51                     | 0.41              |
| 4:CE:21:SER:HA    | 4:CE:29:ILE:O     | 2.20                     | 0.41              |
| 7:CH:9:MET:HE1    | 7:CH:35:ILE:HB    | 2.03                     | 0.41              |
| 7:CH:17:GLN:NE2   | 7:CH:69:ALA:HB1   | 2.36                     | 0.41              |
| 8:CI:35:GLU:O     | 8:CI:39:GLY:HA2   | 2.21                     | 0.41              |
| 8:CI:44:ARG:C     | 8:CI:46:VAL:N     | 2.78                     | 0.41              |
| 8:CI:94:ARG:HH11  | 8:CI:98:ARG:NH1   | 2.19                     | 0.41              |
| 13:CN:29:ILE:HB   | 13:CN:44:VAL:HG21 | 2.03                     | 0.41              |
| 13:CN:56:PRO:C    | 13:CN:58:ARG:H    | 2.29                     | 0.41              |
| 16:CQ:56:ASP:HA   | 16:CQ:81:ALA:HA   | 2.03                     | 0.41              |
| 17:CR:47:ARG:HH12 | 17:CR:49:LYS:H    | 1.69                     | 0.41              |
| 19:CT:38:ILE:HA   | 19:CT:85:LEU:HD22 | 2.02                     | 0.41              |
| 20:CB:125:PHE:C   | 20:CB:127:LYS:N   | 2.78                     | 0.41              |
| 22:DA:70:C:H2'    | 22:DA:71:C:H6     | 1.85                     | 0.41              |
| 22:DA:76:G:O2'    | 22:DA:77:U:H5'    | 2.21                     | 0.41              |
| 23:DB:266:G:O4'   | 23:DB:266:G:OP2   | 2.38                     | 0.41              |
| 23:DB:288:U:H2'   | 23:DB:289:G:C8    | 2.56                     | 0.41              |
| 23:DB:349:U:O2    | 23:DB:349:U:H2'   | 2.20                     | 0.41              |
| 23:DB:458:G:O2'   | 23:DB:459:U:OP2   | 2.39                     | 0.41              |
| 23:DB:675:A:N3    | 23:DB:2443:C:O2'  | 2.52                     | 0.41              |
| 23:DB:927:A:H2'   | 23:DB:928:A:C8    | 2.55                     | 0.41              |
| 23:DB:1030:C:O2'  | 23:DB:1031:G:H5'  | 2.21                     | 0.41              |
| 23:DB:1041:G:C2   | 23:DB:1042:G:N7   | 2.88                     | 0.41              |
| 23:DB:1827:U:C2'  | 23:DB:1828:G:H5'  | 2.51                     | 0.41              |
| 23:DB:1831:G:H2'  | 23:DB:1832:C:C6   | 2.56                     | 0.41              |
| 23:DB:2195:U:O2'  | 23:DB:2196:C:H5'  | 2.21                     | 0.41              |
| 23:DB:2308:G:H3'  | 23:DB:2308:G:N3   | 2.35                     | 0.41              |
| 23:DB:2441:U:O2'  | 23:DB:2442:C:H5'  | 2.21                     | 0.41              |
| 23:DB:2693:G:O2'  | 23:DB:2694:G:H5'  | 2.21                     | 0.41              |
| 23:DB:2694:G:O2'  | 23:DB:2695:U:H5'  | 2.21                     | 0.41              |
| 23:DB:2825:G:C2'  | 23:DB:2826:A:H5'  | 2.51                     | 0.41              |
| 24:DV:83:LYS:C    | 24:DV:85:LYS:N    | 2.77                     | 0.41              |
| 25:DC:62:ARG:O    | 25:DC:62:ARG:NE   | 2.53                     | 0.41              |
| 25:DC:63:ILE:HG23 | 25:DC:102:TYR:HD1 | 1.82                     | 0.41              |
| 25:DC:115:ILE:O   | 25:DC:116:GLN:HG3 | 2.21                     | 0.41              |
| 25:DC:144:GLU:HG2 | 25:DC:150:GLY:HA2 | 2.02                     | 0.41              |
| 26:DD:148:GLN:N   | 26:DD:148:GLN:CD  | 2.78                     | 0.41              |
| 26:DD:160:LYS:O   | 26:DD:160:LYS:HG3 | 2.21                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:DD:196:ALA:O    | 26:DD:197:THR:C    | 2.63                     | 0.41              |
| 27:DE:38:GLY:C     | 27:DE:40:ARG:H     | 2.29                     | 0.41              |
| 29:DG:25:ILE:O     | 29:DG:31:GLU:HA    | 2.21                     | 0.41              |
| 29:DG:62:ALA:C     | 29:DG:64:ALA:H     | 2.27                     | 0.41              |
| 29:DG:145:ALA:HA   | 29:DG:148:ARG:HG2  | 2.02                     | 0.41              |
| 30:DH:67:ALA:C     | 30:DH:69:ALA:N     | 2.78                     | 0.41              |
| 30:DH:68:ARG:HE    | 30:DH:71:LYS:CE    | 2.26                     | 0.41              |
| 32:DK:63:VAL:HB    | 32:DK:83:ALA:CB    | 2.51                     | 0.41              |
| 33:DL:25:SER:HB2   | 33:DL:26:GLY:H     | 1.55                     | 0.41              |
| 34:DM:16:ARG:NE    | 34:DM:18:ARG:NH1   | 2.65                     | 0.41              |
| 34:DM:66:ARG:NE    | 34:DM:66:ARG:HA    | 2.35                     | 0.41              |
| 34:DM:112:LEU:HD23 | 34:DM:112:LEU:HA   | 1.89                     | 0.41              |
| 34:DM:114:ARG:C    | 34:DM:116:ALA:H    | 2.28                     | 0.41              |
| 34:DM:124:LEU:O    | 34:DM:124:LEU:HD12 | 2.21                     | 0.41              |
| 35:DN:98:LEU:HD11  | 35:DN:114:GLU:OE2  | 2.20                     | 0.41              |
| 37:DP:7:LEU:HD23   | 37:DP:7:LEU:C      | 2.45                     | 0.41              |
| 37:DP:27:VAL:O     | 37:DP:29:VAL:N     | 2.53                     | 0.41              |
| 37:DP:27:VAL:HB    | 37:DP:86:LYS:O     | 2.22                     | 0.41              |
| 38:DQ:95:ALA:O     | 38:DQ:98:ALA:HB3   | 2.20                     | 0.41              |
| 38:DQ:102:LYS:O    | 38:DQ:106:THR:HG22 | 2.20                     | 0.41              |
| 39:DR:10:LYS:O     | 39:DR:11:GLN:HB2   | 2.21                     | 0.41              |
| 40:DS:2:GLU:C      | 40:DS:3:THR:HG1    | 2.26                     | 0.41              |
| 40:DS:21:ALA:C     | 40:DS:24:ILE:HG12  | 2.46                     | 0.41              |
| 44:DX:31:GLN:NE2   | 44:DX:31:GLN:CA    | 2.83                     | 0.41              |
| 48:D1:49:LYS:HZ2   | 48:D1:49:LYS:C     | 2.29                     | 0.41              |
| 50:D3:25:HIS:O     | 50:D3:26:ALA:C     | 2.64                     | 0.41              |
| 52:DI:8:VAL:HG11   | 52:DI:30:GLN:HG3   | 2.03                     | 0.41              |
| 1:AA:37:U:O2'      | 1:AA:38:G:H5'      | 2.21                     | 0.40              |
| 1:AA:80:A:C2       | 1:AA:81:A:C4       | 3.09                     | 0.40              |
| 1:AA:213:G:C8      | 1:AA:214:C:C5      | 3.08                     | 0.40              |
| 1:AA:276:G:O2'     | 1:AA:277:C:H5'     | 2.21                     | 0.40              |
| 1:AA:415:A:N3      | 1:AA:415:A:O4'     | 2.53                     | 0.40              |
| 1:AA:807:A:O2'     | 25:BC:4:LYS:HB2    | 2.21                     | 0.40              |
| 1:AA:951:G:O2'     | 1:AA:952:U:H5'     | 2.21                     | 0.40              |
| 1:AA:1015:G:O2'    | 1:AA:1016:A:H5'    | 2.20                     | 0.40              |
| 1:AA:1058:G:H2'    | 1:AA:1059:C:O4'    | 2.20                     | 0.40              |
| 1:AA:1072:G:H2'    | 1:AA:1073:U:H6     | 1.86                     | 0.40              |
| 1:AA:1150:A:N6     | 1:AA:1151:A:N6     | 2.69                     | 0.40              |
| 1:AA:1219:A:OP1    | 13:AN:52:ARG:HG2   | 2.20                     | 0.40              |
| 1:AA:1309:G:O2'    | 1:AA:1310:G:H5'    | 2.20                     | 0.40              |
| 1:AA:1386:G:H2'    | 1:AA:1387:G:H8     | 1.85                     | 0.40              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:1462:C:H2'   | 1:AA:1463:U:H6    | 1.86                     | 0.40              |
| 2:AC:110:LEU:HD22 | 2:AC:145:ALA:HB2  | 2.04                     | 0.40              |
| 2:AC:132:ALA:HA   | 2:AC:136:ALA:HB3  | 2.02                     | 0.40              |
| 4:AE:17:VAL:CG2   | 4:AE:34:ALA:HB2   | 2.50                     | 0.40              |
| 6:AG:101:ARG:O    | 6:AG:105:GLU:N    | 2.46                     | 0.40              |
| 9:AJ:48:ARG:HA    | 9:AJ:66:GLU:HA    | 2.03                     | 0.40              |
| 11:AL:56:LEU:H    | 11:AL:56:LEU:CD1  | 2.34                     | 0.40              |
| 13:AN:27:LYS:NZ   | 13:AN:28:ALA:HB2  | 2.36                     | 0.40              |
| 13:AN:92:ILE:HG21 | 13:AN:95:LEU:HD23 | 2.03                     | 0.40              |
| 16:AQ:64:ARG:HG3  | 16:AQ:65:PRO:HD2  | 2.03                     | 0.40              |
| 18:AS:62:THR:HG22 | 18:AS:63:ASP:N    | 2.36                     | 0.40              |
| 20:AB:88:GLN:HE21 | 20:AB:88:GLN:HB2  | 1.65                     | 0.40              |
| 23:BB:175:G:O2'   | 23:BB:176:A:H5'   | 2.21                     | 0.40              |
| 23:BB:298:G:H1'   | 23:BB:340:A:H61   | 1.86                     | 0.40              |
| 23:BB:330:A:N7    | 23:BB:1210:G:H2'  | 2.37                     | 0.40              |
| 23:BB:600:G:H2'   | 23:BB:601:C:H6    | 1.84                     | 0.40              |
| 23:BB:619:G:H3'   | 23:BB:620:G:H21   | 1.86                     | 0.40              |
| 23:BB:691:C:H1'   | 25:BC:42:ARG:NH1  | 2.36                     | 0.40              |
| 23:BB:911:A:N6    | 34:BM:13:HIS:HB3  | 2.36                     | 0.40              |
| 23:BB:949:G:O2'   | 23:BB:950:G:H5'   | 2.21                     | 0.40              |
| 23:BB:1446:C:H2'  | 23:BB:1447:C:H6   | 1.86                     | 0.40              |
| 23:BB:1537:G:C2'  | 23:BB:1538:G:H5'  | 2.51                     | 0.40              |
| 23:BB:1765:U:O2'  | 23:BB:1766:G:H5'  | 2.19                     | 0.40              |
| 23:BB:1998:A:OP2  | 26:BD:141:ARG:NH2 | 2.54                     | 0.40              |
| 23:BB:2221:G:H2'  | 23:BB:2222:C:C6   | 2.57                     | 0.40              |
| 23:BB:2285:C:N4   | 48:B1:24:LYS:NZ   | 2.69                     | 0.40              |
| 23:BB:2306:C:H1'  | 28:BF:132:ARG:NH2 | 2.37                     | 0.40              |
| 23:BB:2347:C:OP2  | 50:B3:37:THR:HG21 | 2.21                     | 0.40              |
| 23:BB:2408:U:H2'  | 23:BB:2409:G:C8   | 2.55                     | 0.40              |
| 23:BB:2595:G:N2   | 23:BB:2597:G:H3'  | 2.37                     | 0.40              |
| 23:BB:2756:U:H5'  | 51:B4:18:LYS:NZ   | 2.36                     | 0.40              |
| 24:BV:44:HIS:HE2  | 24:BV:85:LYS:CB   | 2.34                     | 0.40              |
| 25:BC:67:LYS:O    | 25:BC:68:ARG:CB   | 2.66                     | 0.40              |
| 25:BC:229:HIS:O   | 25:BC:231:HIS:N   | 2.40                     | 0.40              |
| 26:BD:68:PHE:O    | 26:BD:70:LYS:N    | 2.46                     | 0.40              |
| 26:BD:170:VAL:CG1 | 26:BD:171:THR:H   | 2.13                     | 0.40              |
| 27:BE:16:GLU:O    | 27:BE:17:THR:C    | 2.63                     | 0.40              |
| 27:BE:152:GLU:H   | 27:BE:171:ASP:CG  | 2.29                     | 0.40              |
| 29:BG:6:ALA:H     | 29:BG:7:PRO:CD    | 2.34                     | 0.40              |
| 30:BH:89:LYS:O    | 30:BH:90:LEU:HD12 | 2.21                     | 0.40              |
| 33:BL:38:GLN:O    | 33:BL:39:LYS:C    | 2.65                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:BL:106:GLU:HG2 | 33:BL:107:PHE:N   | 2.36                     | 0.40              |
| 34:BM:82:MET:O    | 34:BM:84:LYS:HG3  | 2.21                     | 0.40              |
| 34:BM:96:ILE:O    | 34:BM:97:GLN:HG3  | 2.21                     | 0.40              |
| 35:BN:28:LEU:HD22 | 35:BN:48:VAL:HG11 | 2.03                     | 0.40              |
| 35:BN:110:MET:O   | 35:BN:111:ALA:HB3 | 2.20                     | 0.40              |
| 37:BP:2:ASN:N     | 37:BP:2:ASN:ND2   | 2.61                     | 0.40              |
| 37:BP:86:LYS:C    | 37:BP:87:ARG:HG3  | 2.46                     | 0.40              |
| 38:BQ:20:ALA:O    | 38:BQ:21:LYS:C    | 2.63                     | 0.40              |
| 40:BS:24:ILE:O    | 40:BS:25:ARG:HB2  | 2.20                     | 0.40              |
| 42:BU:10:VAL:HG11 | 42:BU:25:LYS:HZ3  | 1.86                     | 0.40              |
| 42:BU:11:ILE:C    | 42:BU:69:VAL:HB   | 2.46                     | 0.40              |
| 42:BU:69:VAL:CG1  | 42:BU:77:GLY:H    | 2.34                     | 0.40              |
| 44:BX:36:GLN:OE1  | 44:BX:37:LEU:HG   | 2.22                     | 0.40              |
| 47:B0:39:ARG:HG2  | 47:B0:39:ARG:NH1  | 2.36                     | 0.40              |
| 50:B3:9:ALA:C     | 50:B3:11:LYS:N    | 2.79                     | 0.40              |
| 52:BI:17:ALA:C    | 52:BI:19:PRO:HD2  | 2.46                     | 0.40              |
| 1:CA:401:C:H2'    | 1:CA:402:G:H8     | 1.86                     | 0.40              |
| 1:CA:442:G:H2'    | 1:CA:443:C:H6     | 1.84                     | 0.40              |
| 1:CA:651:C:O2'    | 1:CA:652:U:H5'    | 2.21                     | 0.40              |
| 1:CA:656:G:O2'    | 1:CA:657:U:H5'    | 2.21                     | 0.40              |
| 1:CA:977:A:H3'    | 1:CA:1362:A:N6    | 2.32                     | 0.40              |
| 1:CA:1271:A:H2'   | 1:CA:1272:G:H8    | 1.86                     | 0.40              |
| 1:CA:1526:G:H2'   | 1:CA:1527:U:H6    | 1.85                     | 0.40              |
| 1:CA:1530:G:H2'   | 1:CA:1531:A:C8    | 2.55                     | 0.40              |
| 8:CI:94:ARG:O     | 8:CI:95:SER:C     | 2.64                     | 0.40              |
| 9:CJ:57:VAL:HG13  | 9:CJ:58:ASN:N     | 2.36                     | 0.40              |
| 10:CK:67:GLU:HG3  | 10:CK:68:ARG:N    | 2.36                     | 0.40              |
| 11:CL:56:LEU:HD12 | 11:CL:60:PHE:CB   | 2.50                     | 0.40              |
| 15:CP:54:LEU:HD22 | 15:CP:80:LYS:NZ   | 2.36                     | 0.40              |
| 16:CQ:17:GLU:C    | 16:CQ:19:SER:N    | 2.79                     | 0.40              |
| 18:CS:9:PHE:O     | 18:CS:10:ILE:HG23 | 2.21                     | 0.40              |
| 19:CT:38:ILE:HD11 | 19:CT:82:ILE:CG2  | 2.47                     | 0.40              |
| 20:CB:26:MET:SD   | 20:CB:192:PRO:HD3 | 2.61                     | 0.40              |
| 20:CB:77:GLU:O    | 20:CB:80:LYS:HG2  | 2.21                     | 0.40              |
| 22:DA:49:C:H5''   | 36:DO:101:GLY:HA3 | 2.03                     | 0.40              |
| 22:DA:49:C:C4'    | 36:DO:68:LYS:HZ3  | 2.33                     | 0.40              |
| 22:DA:99:A:N1     | 23:DB:863:A:C4'   | 2.85                     | 0.40              |
| 23:DB:182:A:H1'   | 23:DB:434:U:H5'   | 2.03                     | 0.40              |
| 23:DB:189:G:H2'   | 23:DB:205:G:N2    | 2.37                     | 0.40              |
| 23:DB:848:C:H2'   | 23:DB:849:A:C8    | 2.56                     | 0.40              |
| 23:DB:1019:U:O2'  | 23:DB:1021:A:C2   | 2.70                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:1092:C:C2'  | 23:DB:1093:G:H5'   | 2.51                     | 0.40              |
| 23:DB:1310:G:H1'  | 23:DB:1611:C:H5'   | 2.03                     | 0.40              |
| 23:DB:1549:A:H2'  | 23:DB:1550:C:H6    | 1.84                     | 0.40              |
| 23:DB:1764:C:H2'  | 23:DB:1765:U:C6    | 2.56                     | 0.40              |
| 23:DB:1792:G:O2'  | 23:DB:1793:C:H5'   | 2.21                     | 0.40              |
| 23:DB:1864:U:OP1  | 23:DB:2411:A:H5'   | 2.21                     | 0.40              |
| 23:DB:1936:A:C2   | 23:DB:1943:U:H5    | 2.39                     | 0.40              |
| 23:DB:2215:C:H2'  | 23:DB:2216:G:C8    | 2.56                     | 0.40              |
| 23:DB:2221:G:H2'  | 23:DB:2222:C:H6    | 1.85                     | 0.40              |
| 23:DB:2279:G:N7   | 43:DW:10:ARG:HG3   | 2.36                     | 0.40              |
| 23:DB:2389:G:H5'' | 23:DB:2390:U:O4'   | 2.20                     | 0.40              |
| 23:DB:2405:G:C5'  | 33:DL:70:LYS:HE3   | 2.51                     | 0.40              |
| 24:DV:65:VAL:O    | 24:DV:67:GLY:N     | 2.51                     | 0.40              |
| 25:DC:9:SER:OG    | 25:DC:202:ARG:NH2  | 2.55                     | 0.40              |
| 25:DC:68:ARG:HH21 | 25:DC:190:THR:HG23 | 1.83                     | 0.40              |
| 25:DC:122:ALA:O   | 25:DC:124:LYS:HG2  | 2.21                     | 0.40              |
| 25:DC:168:GLY:C   | 25:DC:170:TYR:N    | 2.79                     | 0.40              |
| 26:DD:79:LEU:CG   | 26:DD:80:TRP:N     | 2.83                     | 0.40              |
| 31:DJ:33:ALA:O    | 31:DJ:36:LEU:HB2   | 2.20                     | 0.40              |
| 32:DK:43:ILE:CD1  | 32:DK:58:LEU:HD21  | 2.50                     | 0.40              |
| 33:DL:135:ILE:C   | 33:DL:137:ALA:N    | 2.78                     | 0.40              |
| 34:DM:6:ARG:C     | 34:DM:8:LYS:N      | 2.79                     | 0.40              |
| 36:DO:15:ARG:HH12 | 43:DW:76:ARG:HD2   | 1.86                     | 0.40              |
| 37:DP:50:ARG:HD2  | 37:DP:99:LEU:HB3   | 2.03                     | 0.40              |
| 39:DR:39:LEU:HG   | 39:DR:62:GLU:HG2   | 2.02                     | 0.40              |
| 39:DR:73:LYS:HD2  | 39:DR:73:LYS:H     | 1.85                     | 0.40              |
| 39:DR:76:LYS:CE   | 39:DR:90:ARG:HD3   | 2.52                     | 0.40              |
| 41:DT:12:ARG:HG2  | 41:DT:13:ALA:H     | 1.85                     | 0.40              |
| 42:DU:17:ASP:CG   | 42:DU:20:LYS:HB2   | 2.46                     | 0.40              |
| 42:DU:43:LYS:NZ   | 42:DU:43:LYS:CB    | 2.84                     | 0.40              |
| 42:DU:44:HIS:O    | 42:DU:46:LYS:HD2   | 2.21                     | 0.40              |
| 42:DU:96:LYS:HE2  | 42:DU:96:LYS:HB2   | 1.94                     | 0.40              |
| 43:DW:24:ARG:HE   | 43:DW:58:LEU:HB2   | 1.86                     | 0.40              |
| 43:DW:48:ALA:HA   | 43:DW:54:ARG:N     | 2.35                     | 0.40              |
| 48:D1:4:ILE:O     | 48:D1:4:ILE:HG13   | 2.21                     | 0.40              |
| 1:AA:175:C:H2'    | 1:AA:176:C:H6      | 1.85                     | 0.40              |
| 1:AA:239:U:C5'    | 1:AA:239:U:C6      | 2.97                     | 0.40              |
| 1:AA:471:U:O2'    | 1:AA:472:U:H5'     | 2.21                     | 0.40              |
| 1:AA:669:G:O2'    | 1:AA:670:G:H5'     | 2.22                     | 0.40              |
| 1:AA:1343:G:H1'   | 8:AI:122:ARG:NH1   | 2.35                     | 0.40              |
| 3:AD:153:ARG:HG2  | 3:AD:153:ARG:NH1   | 2.36                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:AD:187:ARG:HG3  | 3:AD:187:ARG:HH11 | 1.85                     | 0.40              |
| 6:AG:132:THR:HG23 | 6:AG:135:LYS:NZ   | 2.35                     | 0.40              |
| 7:AH:26:MET:CB    | 7:AH:27:PRO:HD2   | 2.49                     | 0.40              |
| 7:AH:76:ARG:HD3   | 7:AH:79:ARG:HB3   | 2.02                     | 0.40              |
| 11:AL:31:GLY:O    | 11:AL:78:VAL:HG13 | 2.22                     | 0.40              |
| 12:AM:106:ARG:HD3 | 12:AM:109:LYS:HD2 | 2.03                     | 0.40              |
| 14:AO:82:GLU:OE1  | 14:AO:82:GLU:HA   | 2.21                     | 0.40              |
| 14:AO:87:ARG:C    | 14:AO:88:ARG:HG2  | 2.46                     | 0.40              |
| 16:AQ:4:ILE:HD12  | 16:AQ:5:ARG:H     | 1.85                     | 0.40              |
| 16:AQ:10:ARG:NE   | 16:AQ:56:ASP:O    | 2.54                     | 0.40              |
| 18:AS:18:VAL:HG13 | 18:AS:19:GLU:N    | 2.36                     | 0.40              |
| 18:AS:29:PRO:C    | 18:AS:30:LEU:HD22 | 2.46                     | 0.40              |
| 19:AT:60:GLN:C    | 19:AT:62:ALA:N    | 2.78                     | 0.40              |
| 22:BA:30:C:H2'    | 22:BA:31:C:H5'    | 2.03                     | 0.40              |
| 22:BA:81:G:H2'    | 22:BA:82:U:H6     | 1.85                     | 0.40              |
| 23:BB:102:U:H4'   | 23:BB:103:A:OP2   | 2.13                     | 0.40              |
| 23:BB:123:G:O2'   | 23:BB:124:G:H5'   | 2.21                     | 0.40              |
| 23:BB:135:U:H6    | 23:BB:135:U:O5'   | 2.04                     | 0.40              |
| 23:BB:154:U:O2'   | 23:BB:155:A:H5'   | 2.22                     | 0.40              |
| 23:BB:428:A:H2'   | 23:BB:429:A:O4'   | 2.21                     | 0.40              |
| 23:BB:622:G:H2'   | 23:BB:623:C:C6    | 2.56                     | 0.40              |
| 23:BB:975:A:N6    | 23:BB:989:G:H1'   | 2.37                     | 0.40              |
| 23:BB:977:G:H5'   | 23:BB:1155:A:H4'  | 2.03                     | 0.40              |
| 23:BB:1017:G:H2'  | 23:BB:1018:U:H6   | 1.86                     | 0.40              |
| 23:BB:1185:G:H5'' | 23:BB:1186:G:OP1  | 2.21                     | 0.40              |
| 23:BB:1411:U:O2'  | 23:BB:1412:U:H5'  | 2.21                     | 0.40              |
| 23:BB:1719:G:O2'  | 23:BB:1720:U:H5'  | 2.22                     | 0.40              |
| 23:BB:2311:A:H1'  | 28:BF:76:PHE:HE1  | 1.87                     | 0.40              |
| 23:BB:2313:C:H2'  | 23:BB:2314:A:H8   | 1.84                     | 0.40              |
| 23:BB:2485:G:H1'  | 34:BM:118:LYS:HZ3 | 1.86                     | 0.40              |
| 23:BB:2732:G:H3'  | 23:BB:2733:A:H5'  | 2.02                     | 0.40              |
| 23:BB:2799:A:H4'  | 23:BB:2800:A:C8   | 2.56                     | 0.40              |
| 23:BB:2838:G:C4   | 23:BB:2839:G:C8   | 3.10                     | 0.40              |
| 24:BV:9:ARG:HH22  | 24:BV:27:PRO:HB3  | 1.86                     | 0.40              |
| 24:BV:76:ASP:CG   | 24:BV:77:VAL:N    | 2.78                     | 0.40              |
| 25:BC:175:LEU:H   | 25:BC:175:LEU:HG  | 1.74                     | 0.40              |
| 25:BC:206:LYS:O   | 25:BC:207:ALA:C   | 2.64                     | 0.40              |
| 25:BC:216:ARG:O   | 25:BC:218:THR:N   | 2.53                     | 0.40              |
| 25:BC:220:ARG:HG3 | 25:BC:220:ARG:NH1 | 2.36                     | 0.40              |
| 25:BC:248:GLY:C   | 25:BC:250:GLN:N   | 2.78                     | 0.40              |
| 25:BC:259:ASN:O   | 25:BC:261:ARG:HG2 | 2.21                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:BD:132:ALA:O    | 26:BD:136:ASN:CG   | 2.64                     | 0.40              |
| 26:BD:192:ALA:O    | 26:BD:193:VAL:HG12 | 2.22                     | 0.40              |
| 28:BF:12:VAL:CG1   | 28:BF:27:VAL:HG21  | 2.49                     | 0.40              |
| 28:BF:13:LYS:HE2   | 28:BF:24:VAL:HG12  | 2.03                     | 0.40              |
| 28:BF:109:ARG:CG   | 28:BF:136:ILE:HG13 | 2.50                     | 0.40              |
| 29:BG:26:LYS:HE2   | 29:BG:26:LYS:HB3   | 1.85                     | 0.40              |
| 29:BG:131:VAL:HG13 | 29:BG:133:LYS:CE   | 2.49                     | 0.40              |
| 30:BH:28:ASN:O     | 30:BH:29:PHE:HB2   | 2.21                     | 0.40              |
| 31:BJ:23:LYS:HD2   | 31:BJ:23:LYS:N     | 2.33                     | 0.40              |
| 31:BJ:60:ASP:OD1   | 31:BJ:97:PRO:HG2   | 2.21                     | 0.40              |
| 32:BK:76:VAL:O     | 37:BP:74:GLN:HG2   | 2.21                     | 0.40              |
| 33:BL:65:GLY:O     | 33:BL:66:PHE:HB3   | 2.20                     | 0.40              |
| 33:BL:94:THR:CG2   | 33:BL:95:LEU:HD12  | 2.37                     | 0.40              |
| 34:BM:81:ARG:O     | 34:BM:81:ARG:HG3   | 2.21                     | 0.40              |
| 34:BM:132:THR:C    | 34:BM:134:THR:H    | 2.28                     | 0.40              |
| 35:BN:73:ASN:N     | 35:BN:73:ASN:ND2   | 2.68                     | 0.40              |
| 36:BO:68:LYS:C     | 36:BO:70:ALA:N     | 2.76                     | 0.40              |
| 37:BP:92:ARG:NH2   | 37:BP:110:LYS:HB3  | 2.36                     | 0.40              |
| 38:BQ:5:ARG:H      | 38:BQ:5:ARG:HD3    | 1.86                     | 0.40              |
| 38:BQ:92:LYS:HG2   | 38:BQ:93:ILE:N     | 2.10                     | 0.40              |
| 40:BS:86:MET:HB3   | 40:BS:94:ASP:HB3   | 2.03                     | 0.40              |
| 42:BU:10:VAL:O     | 42:BU:11:ILE:HD13  | 2.22                     | 0.40              |
| 45:BY:6:ILE:O      | 45:BY:6:ILE:HG12   | 2.20                     | 0.40              |
| 48:B1:35:LEU:O     | 48:B1:35:LEU:HG    | 2.21                     | 0.40              |
| 49:B2:8:SER:OG     | 49:B2:11:LYS:HB2   | 2.21                     | 0.40              |
| 50:B3:7:ARG:O      | 50:B3:8:GLY:C      | 2.63                     | 0.40              |
| 1:CA:99:C:H2'      | 55:CA:1943:HOH:O   | 2.21                     | 0.40              |
| 1:CA:119:A:H4'     | 1:CA:120:A:O4'     | 2.21                     | 0.40              |
| 1:CA:123:U:H2'     | 1:CA:124:C:H6      | 1.86                     | 0.40              |
| 1:CA:144:G:H2'     | 1:CA:145:G:C8      | 2.56                     | 0.40              |
| 1:CA:213:G:C8      | 1:CA:214:C:C5      | 3.09                     | 0.40              |
| 1:CA:374:A:OP1     | 1:CA:452:A:N1      | 2.55                     | 0.40              |
| 1:CA:666:G:H5'     | 1:CA:726:C:H1'     | 2.03                     | 0.40              |
| 1:CA:1011:C:H2'    | 1:CA:1012:A:H8     | 1.85                     | 0.40              |
| 1:CA:1209:C:O2'    | 1:CA:1210:C:H5'    | 2.21                     | 0.40              |
| 1:CA:1446:A:N6     | 1:CA:1447:A:N6     | 2.69                     | 0.40              |
| 4:CE:146:MET:HG2   | 4:CE:147:ASN:N     | 2.36                     | 0.40              |
| 6:CG:22:LEU:O      | 6:CG:23:ALA:C      | 2.63                     | 0.40              |
| 6:CG:132:THR:O     | 6:CG:135:LYS:HB3   | 2.21                     | 0.40              |
| 7:CH:54:THR:HG23   | 7:CH:55:LYS:HE2    | 2.02                     | 0.40              |
| 13:CN:68:ARG:HH12  | 13:CN:71:GLY:H     | 1.67                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:CQ:56:ASP:OD1   | 16:CQ:80:LYS:HA    | 2.21                     | 0.40              |
| 18:CS:39:ILE:HA    | 18:CS:43:MET:SD    | 2.60                     | 0.40              |
| 23:DB:553:G:C2'    | 23:DB:554:U:H5'    | 2.52                     | 0.40              |
| 23:DB:1228:G:O2'   | 23:DB:1229:C:H5'   | 2.21                     | 0.40              |
| 23:DB:1266:G:OP2   | 47:D0:12:ARG:CZ    | 2.69                     | 0.40              |
| 23:DB:1708:C:H2'   | 23:DB:1709:U:C6    | 2.57                     | 0.40              |
| 23:DB:1723:G:N7    | 23:DB:1724:G:N7    | 2.69                     | 0.40              |
| 23:DB:1856:U:C2'   | 23:DB:1857:G:H5'   | 2.52                     | 0.40              |
| 23:DB:1945:G:H2'   | 23:DB:1946:U:H6    | 1.82                     | 0.40              |
| 23:DB:2186:G:H2'   | 23:DB:2187:U:O4'   | 2.21                     | 0.40              |
| 23:DB:2250:G:O6    | 34:DM:82:MET:HE3   | 2.21                     | 0.40              |
| 23:DB:2673:G:H2'   | 23:DB:2674:G:H8    | 1.86                     | 0.40              |
| 23:DB:2820:A:O3'   | 35:DN:2:ARG:NH2    | 2.53                     | 0.40              |
| 25:DC:160:TYR:CD2  | 25:DC:193:GLU:HG2  | 2.56                     | 0.40              |
| 26:DD:60:VAL:CG2   | 26:DD:63:PRO:HG2   | 2.43                     | 0.40              |
| 27:DE:193:VAL:C    | 27:DE:195:GLN:N    | 2.78                     | 0.40              |
| 28:DF:157:THR:HG22 | 28:DF:159:ALA:H    | 1.87                     | 0.40              |
| 31:DJ:23:LYS:HE2   | 31:DJ:23:LYS:HB3   | 1.87                     | 0.40              |
| 32:DK:107:LEU:C    | 32:DK:109:SER:H    | 2.28                     | 0.40              |
| 34:DM:5:LYS:O      | 34:DM:7:THR:HG23   | 2.21                     | 0.40              |
| 34:DM:42:THR:O     | 34:DM:45:GLN:HB2   | 2.22                     | 0.40              |
| 34:DM:71:LYS:HG2   | 34:DM:71:LYS:H     | 1.58                     | 0.40              |
| 34:DM:102:LEU:N    | 34:DM:102:LEU:HD22 | 2.35                     | 0.40              |
| 36:DO:109:ALA:HA   | 36:DO:112:GLU:CG   | 2.51                     | 0.40              |
| 37:DP:36:LYS:CG    | 37:DP:37:LYS:H     | 2.33                     | 0.40              |
| 38:DQ:101:ASP:O    | 38:DQ:105:PHE:HB2  | 2.21                     | 0.40              |
| 39:DR:82:HIS:C     | 39:DR:84:ARG:H     | 2.28                     | 0.40              |
| 40:DS:64:ALA:HA    | 40:DS:110:ARG:NH2  | 2.36                     | 0.40              |
| 41:DT:7:LEU:H      | 41:DT:7:LEU:CD2    | 2.33                     | 0.40              |
| 41:DT:15:HIS:HB3   | 41:DT:31:VAL:HG11  | 2.03                     | 0.40              |
| 43:DW:36:ILE:HG12  | 43:DW:69:GLU:OE2   | 2.21                     | 0.40              |
| 43:DW:67:LYS:HG2   | 43:DW:71:LYS:N     | 2.36                     | 0.40              |
| 44:DX:26:PHE:N     | 44:DX:26:PHE:CD1   | 2.89                     | 0.40              |
| 44:DX:41:HIS:CE1   | 44:DX:43:LEU:HD23  | 2.56                     | 0.40              |
| 46:DZ:49:ARG:NH1   | 46:DZ:49:ARG:HB2   | 2.36                     | 0.40              |
| 51:D4:28:SER:O     | 51:D4:29:ALA:HB3   | 2.21                     | 0.40              |
| 52:DI:17:ALA:C     | 52:DI:19:PRO:CD    | 2.93                     | 0.40              |
| 1:AA:80:A:C2       | 1:AA:81:A:H1'      | 2.57                     | 0.40              |
| 1:AA:82:G:H3'      | 1:AA:83:C:H4'      | 2.02                     | 0.40              |
| 1:AA:258:G:N2      | 1:AA:259:G:H1'     | 2.37                     | 0.40              |
| 1:AA:619:U:O2      | 3:AD:129:VAL:HA    | 2.22                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:672:U:H2'    | 1:AA:673:A:H8     | 1.83                     | 0.40              |
| 1:AA:828:U:H2'    | 1:AA:829:G:O5'    | 2.21                     | 0.40              |
| 1:AA:977:A:N1     | 1:AA:1224:U:O5'   | 2.54                     | 0.40              |
| 1:AA:978:A:H5'    | 1:AA:1362:A:H62   | 1.83                     | 0.40              |
| 1:AA:1080:A:H2'   | 1:AA:1081:A:H5'   | 2.03                     | 0.40              |
| 1:AA:1237:C:C4'   | 1:AA:1334:G:N2    | 2.85                     | 0.40              |
| 1:AA:1340:A:H2'   | 1:AA:1341:U:C6    | 2.57                     | 0.40              |
| 2:AC:205:GLU:HB2  | 2:AC:206:ILE:H    | 1.59                     | 0.40              |
| 5:AF:9:MET:HE1    | 17:AR:64:LEU:CA   | 2.51                     | 0.40              |
| 7:AH:30:LYS:NZ    | 7:AH:30:LYS:CA    | 2.78                     | 0.40              |
| 11:AL:19:ASN:HB2  | 11:AL:93:ARG:CZ   | 2.52                     | 0.40              |
| 12:AM:65:GLU:O    | 12:AM:66:GLY:C    | 2.64                     | 0.40              |
| 13:AN:17:ASP:C    | 13:AN:19:TYR:N    | 2.79                     | 0.40              |
| 18:AS:4:LEU:N     | 18:AS:5:LYS:HE3   | 2.35                     | 0.40              |
| 20:AB:98:GLY:HA2  | 20:AB:101:THR:CG2 | 2.51                     | 0.40              |
| 23:BB:20:C:O2'    | 23:BB:21:A:H5'    | 2.21                     | 0.40              |
| 23:BB:143:C:C2'   | 23:BB:144:A:C8    | 3.04                     | 0.40              |
| 23:BB:442:G:N2    | 23:BB:444:C:C2    | 2.90                     | 0.40              |
| 23:BB:515:A:H3'   | 23:BB:516:C:C6    | 2.56                     | 0.40              |
| 23:BB:878:A:OP1   | 23:BB:899:A:N6    | 2.53                     | 0.40              |
| 23:BB:1036:G:O2'  | 23:BB:1037:G:H5'  | 2.21                     | 0.40              |
| 23:BB:1050:A:C2   | 23:BB:1051:G:H1'  | 2.57                     | 0.40              |
| 23:BB:1254:A:OP2  | 23:BB:1256:G:H8   | 2.04                     | 0.40              |
| 23:BB:1306:C:O2'  | 23:BB:1307:A:H5'  | 2.22                     | 0.40              |
| 23:BB:1541:C:H2'  | 23:BB:1542:U:H6   | 1.85                     | 0.40              |
| 23:BB:1695:G:N7   | 25:BC:14:HIS:HD2  | 2.19                     | 0.40              |
| 23:BB:1758:U:N3   | 23:BB:2696:U:H5'  | 2.35                     | 0.40              |
| 23:BB:1788:C:O2'  | 23:BB:1789:A:H5'  | 2.21                     | 0.40              |
| 23:BB:2528:U:P    | 51:B4:31:PRO:HG2  | 2.61                     | 0.40              |
| 23:BB:2574:G:O2'  | 26:BD:148:GLN:NE2 | 2.55                     | 0.40              |
| 23:BB:2887:A:O2'  | 23:BB:2888:C:H5'  | 2.21                     | 0.40              |
| 25:BC:190:THR:C   | 25:BC:192:GLY:H   | 2.29                     | 0.40              |
| 25:BC:228:ASP:OD1 | 25:BC:228:ASP:N   | 2.53                     | 0.40              |
| 26:BD:33:ARG:HG3  | 26:BD:34:VAL:N    | 2.31                     | 0.40              |
| 26:BD:43:ASP:CG   | 26:BD:44:GLY:H    | 2.30                     | 0.40              |
| 27:BE:37:ALA:O    | 27:BE:93:SER:HA   | 2.21                     | 0.40              |
| 27:BE:44:ARG:C    | 27:BE:46:GLN:N    | 2.75                     | 0.40              |
| 27:BE:52:VAL:HG22 | 27:BE:53:THR:N    | 2.29                     | 0.40              |
| 30:BH:82:SER:O    | 30:BH:90:LEU:HD23 | 2.21                     | 0.40              |
| 31:BJ:73:VAL:HG21 | 31:BJ:75:TYR:OH   | 2.21                     | 0.40              |
| 33:BL:69:ARG:HH11 | 33:BL:69:ARG:HG2  | 1.86                     | 0.40              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:BL:123:ARG:O   | 33:BL:126:ARG:HG3  | 2.21                     | 0.40              |
| 34:BM:33:LEU:H    | 34:BM:101:VAL:HG22 | 1.81                     | 0.40              |
| 34:BM:71:LYS:O    | 34:BM:73:ILE:HD12  | 2.22                     | 0.40              |
| 35:BN:65:LEU:HD12 | 35:BN:65:LEU:HA    | 1.93                     | 0.40              |
| 36:BO:34:HIS:ND1  | 36:BO:34:HIS:N     | 2.69                     | 0.40              |
| 37:BP:51:ASN:ND2  | 37:BP:97:TYR:CE2   | 2.90                     | 0.40              |
| 37:BP:67:GLU:HG3  | 37:BP:67:GLU:O     | 2.20                     | 0.40              |
| 38:BQ:93:ILE:HG23 | 38:BQ:94:LEU:N     | 2.31                     | 0.40              |
| 38:BQ:94:LEU:HB3  | 39:BR:13:ARG:HG2   | 2.03                     | 0.40              |
| 39:BR:90:ARG:NH1  | 39:BR:91:GLN:C     | 2.79                     | 0.40              |
| 40:BS:3:THR:HG23  | 40:BS:107:VAL:O    | 2.22                     | 0.40              |
| 41:BT:12:ARG:NH2  | 44:BX:29:ARG:NH1   | 2.59                     | 0.40              |
| 41:BT:24:MET:HG3  | 41:BT:28:ASN:HA    | 2.02                     | 0.40              |
| 41:BT:68:LYS:HA   | 41:BT:75:GLY:HA3   | 2.03                     | 0.40              |
| 42:BU:43:LYS:HE2  | 42:BU:45:GLN:HG2   | 2.03                     | 0.40              |
| 44:BX:14:LEU:HD21 | 44:BX:57:LEU:HD22  | 2.02                     | 0.40              |
| 48:B1:51:ALA:CB   | 48:B1:52:LYS:HD2   | 2.52                     | 0.40              |
| 50:B3:22:LYS:HA   | 50:B3:22:LYS:HD3   | 1.88                     | 0.40              |
| 1:CA:412:A:H1'    | 1:CA:413:G:C8      | 2.45                     | 0.40              |
| 1:CA:471:U:O2'    | 1:CA:472:U:H5'     | 2.22                     | 0.40              |
| 1:CA:552:U:H5'    | 11:CL:82:ARG:HH11  | 1.87                     | 0.40              |
| 1:CA:598:U:C2     | 1:CA:599:C:C5      | 3.09                     | 0.40              |
| 1:CA:612:C:H2'    | 1:CA:613:C:C6      | 2.56                     | 0.40              |
| 1:CA:619:U:O2     | 3:CD:129:VAL:HG13  | 2.22                     | 0.40              |
| 1:CA:846:G:H5'    | 1:CA:847:G:OP2     | 2.21                     | 0.40              |
| 1:CA:1046:A:H2'   | 1:CA:1047:G:O4'    | 2.21                     | 0.40              |
| 1:CA:1074:G:H2'   | 1:CA:1075:U:C6     | 2.53                     | 0.40              |
| 1:CA:1099:G:H2'   | 1:CA:1100:C:O4'    | 2.21                     | 0.40              |
| 1:CA:1125:U:O2    | 1:CA:1126:U:H6     | 2.04                     | 0.40              |
| 1:CA:1321:U:H2'   | 1:CA:1322:C:C5     | 2.56                     | 0.40              |
| 1:CA:1326:U:H2'   | 1:CA:1327:C:H6     | 1.86                     | 0.40              |
| 2:CC:85:LYS:O     | 2:CC:89:VAL:HG13   | 2.21                     | 0.40              |
| 2:CC:133:MET:HE1  | 2:CC:165:GLU:HB3   | 2.03                     | 0.40              |
| 3:CD:167:PRO:CG   | 3:CD:170:LEU:HD11  | 2.35                     | 0.40              |
| 3:CD:187:ARG:HE   | 3:CD:196:GLU:CD    | 2.29                     | 0.40              |
| 4:CE:52:ALA:C     | 4:CE:54:GLU:H      | 2.28                     | 0.40              |
| 6:CG:49:LEU:C     | 6:CG:49:LEU:HD23   | 2.47                     | 0.40              |
| 7:CH:7:ALA:O      | 7:CH:11:THR:HG23   | 2.21                     | 0.40              |
| 11:CL:24:GLU:HB2  | 11:CL:26:CYS:SG    | 2.61                     | 0.40              |
| 11:CL:62:VAL:HG11 | 11:CL:94:TYR:HE1   | 1.87                     | 0.40              |
| 12:CM:13:HIS:HA   | 12:CM:43:LYS:HA    | 2.02                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:CM:21:ILE:O    | 12:CM:23:GLY:N     | 2.55                     | 0.40              |
| 13:CN:9:GLU:O     | 13:CN:13:VAL:HG23  | 2.20                     | 0.40              |
| 14:CO:16:ARG:CZ   | 14:CO:76:ARG:NH2   | 2.85                     | 0.40              |
| 18:CS:35:ARG:NH2  | 18:CS:74:ALA:HB3   | 2.37                     | 0.40              |
| 18:CS:39:ILE:HG12 | 18:CS:68:HIS:O     | 2.20                     | 0.40              |
| 21:CU:3:ILE:HD11  | 21:CU:19:LYS:HD3   | 2.04                     | 0.40              |
| 22:DA:40:U:C2     | 22:DA:43:C:H5''    | 2.56                     | 0.40              |
| 23:DB:7:G:H2'     | 23:DB:8:C:O4'      | 2.21                     | 0.40              |
| 23:DB:137:U:C5    | 23:DB:138:U:C4     | 3.09                     | 0.40              |
| 23:DB:242:G:H5'   | 50:D3:61:LEU:HD23  | 2.04                     | 0.40              |
| 23:DB:622:G:H2'   | 23:DB:623:C:C6     | 2.56                     | 0.40              |
| 23:DB:689:A:H2'   | 23:DB:690:G:H8     | 1.85                     | 0.40              |
| 23:DB:876:C:H3'   | 23:DB:877:A:C4'    | 2.52                     | 0.40              |
| 23:DB:1299:G:C5'  | 23:DB:1301:A:H1'   | 2.51                     | 0.40              |
| 23:DB:1506:U:H2'  | 23:DB:1507:C:H6    | 1.87                     | 0.40              |
| 23:DB:1658:C:OP1  | 26:DD:136:ASN:CG   | 2.64                     | 0.40              |
| 23:DB:1989:G:H2'  | 23:DB:1990:C:O4'   | 2.21                     | 0.40              |
| 23:DB:2143:C:H3'  | 23:DB:2144:G:C8    | 2.48                     | 0.40              |
| 23:DB:2150:C:H2'  | 23:DB:2151:U:H6    | 1.85                     | 0.40              |
| 23:DB:2786:U:O2   | 26:DD:62:LYS:HB3   | 2.22                     | 0.40              |
| 25:DC:22:GLU:HB2  | 25:DC:202:ARG:NE   | 2.37                     | 0.40              |
| 25:DC:51:ARG:O    | 25:DC:52:HIS:O     | 2.39                     | 0.40              |
| 26:DD:72:GLY:O    | 26:DD:91:THR:OG1   | 2.38                     | 0.40              |
| 26:DD:81:GLU:O    | 26:DD:82:PHE:CB    | 2.69                     | 0.40              |
| 26:DD:87:GLY:HA3  | 26:DD:89:GLU:OE1   | 2.21                     | 0.40              |
| 26:DD:175:LEU:HB3 | 26:DD:189:VAL:HG12 | 2.02                     | 0.40              |
| 27:DE:132:LYS:C   | 27:DE:134:LEU:HD13 | 2.46                     | 0.40              |
| 28:DF:83:PRO:O    | 28:DF:84:ILE:C     | 2.64                     | 0.40              |
| 31:DJ:15:TRP:HB3  | 31:DJ:138:GLN:O    | 2.22                     | 0.40              |
| 31:DJ:124:VAL:O   | 31:DJ:125:TYR:HB2  | 2.20                     | 0.40              |
| 33:DL:39:LYS:H    | 33:DL:39:LYS:NZ    | 2.08                     | 0.40              |
| 34:DM:81:ARG:HB2  | 34:DM:81:ARG:HH11  | 1.86                     | 0.40              |
| 35:DN:81:ASN:O    | 35:DN:85:PRO:HG3   | 2.22                     | 0.40              |
| 36:DO:39:VAL:O    | 36:DO:39:VAL:HG22  | 2.21                     | 0.40              |
| 37:DP:38:ARG:CG   | 37:DP:39:LEU:N     | 2.75                     | 0.40              |
| 37:DP:38:ARG:HD2  | 37:DP:38:ARG:HA    | 1.61                     | 0.40              |
| 38:DQ:30:VAL:O    | 38:DQ:31:TYR:HB2   | 2.21                     | 0.40              |
| 38:DQ:71:ASN:O    | 38:DQ:73:ILE:N     | 2.54                     | 0.40              |
| 41:DT:87:LEU:HD13 | 41:DT:93:LEU:HD13  | 2.02                     | 0.40              |
| 47:D0:41:HIS:HB3  | 47:D0:46:GLY:CA    | 2.51                     | 0.40              |
| 48:D1:33:LEU:HD12 | 48:D1:33:LEU:N     | 2.37                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 50:D3:4:LYS:O     | 50:D3:6:VAL:N     | 2.54                     | 0.40              |
| 51:D4:1:MET:HE1   | 51:D4:35:GLN:HA   | 2.03                     | 0.40              |
| 1:AA:123:U:H2'    | 1:AA:124:C:H6     | 1.86                     | 0.40              |
| 1:AA:201:G:O2'    | 1:AA:202:G:H5'    | 2.21                     | 0.40              |
| 1:AA:438:U:H4'    | 3:AD:119:HIS:HD2  | 1.85                     | 0.40              |
| 1:AA:454:G:H2'    | 1:AA:455:G:H8     | 1.86                     | 0.40              |
| 1:AA:973:G:O2'    | 9:AJ:56:HIS:HA    | 2.21                     | 0.40              |
| 1:AA:1021:A:H2'   | 1:AA:1022:A:C8    | 2.56                     | 0.40              |
| 1:AA:1057:G:H2'   | 1:AA:1058:G:O4'   | 2.21                     | 0.40              |
| 1:AA:1095:U:O2'   | 1:AA:1096:C:H5'   | 2.22                     | 0.40              |
| 1:AA:1238:A:H2    | 1:AA:1241:G:H1'   | 1.85                     | 0.40              |
| 1:AA:1371:G:O3'   | 8:AI:70:GLY:HA3   | 2.20                     | 0.40              |
| 1:AA:1458:G:O3'   | 19:AT:22:SER:HA   | 2.22                     | 0.40              |
| 2:AC:5:HIS:NE2    | 2:AC:7:ASN:HB2    | 2.37                     | 0.40              |
| 2:AC:154:GLY:CA   | 2:AC:163:ARG:H    | 2.33                     | 0.40              |
| 3:AD:84:ASN:O     | 3:AD:88:ASN:ND2   | 2.54                     | 0.40              |
| 8:AI:16:ALA:HB1   | 8:AI:78:ILE:HA    | 2.03                     | 0.40              |
| 14:AO:24:THR:O    | 14:AO:28:VAL:HG23 | 2.21                     | 0.40              |
| 16:AQ:50:ASN:C    | 16:AQ:52:CYS:H    | 2.28                     | 0.40              |
| 18:AS:30:LEU:HD22 | 18:AS:30:LEU:N    | 2.36                     | 0.40              |
| 23:BB:18:U:O2'    | 23:BB:19:A:H5'    | 2.21                     | 0.40              |
| 23:BB:27:G:O2'    | 23:BB:513:A:N6    | 2.54                     | 0.40              |
| 23:BB:116:C:H2'   | 23:BB:117:G:C8    | 2.57                     | 0.40              |
| 23:BB:553:G:H2'   | 23:BB:554:U:C6    | 2.56                     | 0.40              |
| 23:BB:920:A:H2'   | 23:BB:921:C:C6    | 2.55                     | 0.40              |
| 23:BB:1010:A:H4'  | 23:BB:1152:C:O2'  | 2.22                     | 0.40              |
| 23:BB:1018:U:H2'  | 23:BB:1019:U:O4'  | 2.22                     | 0.40              |
| 23:BB:1708:C:H2'  | 23:BB:1709:U:C6   | 2.56                     | 0.40              |
| 23:BB:1893:C:H2'  | 23:BB:1894:C:O4'  | 2.21                     | 0.40              |
| 23:BB:2080:A:H2'  | 23:BB:2081:U:H6   | 1.86                     | 0.40              |
| 23:BB:2155:U:H6   | 23:BB:2155:U:O5'  | 2.05                     | 0.40              |
| 23:BB:2179:C:H2'  | 23:BB:2180:U:C6   | 2.56                     | 0.40              |
| 23:BB:2312:U:H2'  | 23:BB:2313:C:H5'  | 2.03                     | 0.40              |
| 23:BB:2363:G:P    | 50:B3:39:ARG:HD3  | 2.62                     | 0.40              |
| 23:BB:2377:A:H2'  | 23:BB:2378:A:C8   | 2.56                     | 0.40              |
| 23:BB:2444:G:OP1  | 27:BE:62:GLN:NE2  | 2.55                     | 0.40              |
| 23:BB:2822:G:OP1  | 26:BD:166:GLY:CA  | 2.69                     | 0.40              |
| 24:BV:35:GLU:HG3  | 24:BV:93:ARG:NE   | 2.35                     | 0.40              |
| 27:BE:48:THR:CA   | 27:BE:86:ALA:HB1  | 2.51                     | 0.40              |
| 29:BG:40:VAL:CG1  | 29:BG:41:GLU:N    | 2.84                     | 0.40              |
| 29:BG:153:PRO:HG3 | 29:BG:160:GLY:C   | 2.47                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:BH:57:LYS:HA    | 30:BH:61:VAL:HB    | 2.02                     | 0.40              |
| 31:BJ:110:PRO:O    | 31:BJ:111:LYS:HB2  | 2.22                     | 0.40              |
| 33:BL:55:MET:N     | 33:BL:55:MET:SD    | 2.93                     | 0.40              |
| 33:BL:61:LEU:O     | 33:BL:62:PRO:C     | 2.65                     | 0.40              |
| 33:BL:120:VAL:HG12 | 33:BL:138:ALA:HB3  | 2.02                     | 0.40              |
| 35:BN:22:ARG:NE    | 35:BN:69:ARG:HD3   | 2.37                     | 0.40              |
| 35:BN:28:LEU:HG    | 35:BN:34:ILE:CD1   | 2.51                     | 0.40              |
| 36:BO:40:ILE:HD13  | 36:BO:40:ILE:N     | 2.35                     | 0.40              |
| 36:BO:53:THR:O     | 36:BO:54:VAL:C     | 2.64                     | 0.40              |
| 39:BR:41:ILE:HD12  | 39:BR:43:ASN:H     | 1.86                     | 0.40              |
| 39:BR:43:ASN:C     | 39:BR:45:GLU:N     | 2.78                     | 0.40              |
| 40:BS:13:SER:OG    | 40:BS:16:LYS:HD3   | 2.21                     | 0.40              |
| 41:BT:3:ARG:HE     | 41:BT:8:LEU:CD2    | 2.34                     | 0.40              |
| 42:BU:8:ASP:O      | 42:BU:10:VAL:HG13  | 2.21                     | 0.40              |
| 42:BU:13:LEU:O     | 42:BU:15:GLY:N     | 2.54                     | 0.40              |
| 42:BU:25:LYS:CG    | 42:BU:35:VAL:HA    | 2.41                     | 0.40              |
| 42:BU:48:VAL:C     | 42:BU:50:ALA:H     | 2.28                     | 0.40              |
| 43:BW:59:PHE:HE2   | 43:BW:81:ILE:CD1   | 2.35                     | 0.40              |
| 46:BZ:34:LEU:H     | 46:BZ:44:PHE:CB    | 2.34                     | 0.40              |
| 48:B1:10:LEU:HD11  | 48:B1:52:LYS:HD3   | 2.04                     | 0.40              |
| 49:B2:12:ARG:NH1   | 49:B2:44:VAL:O     | 2.55                     | 0.40              |
| 49:B2:42:LEU:HG    | 49:B2:43:THR:H     | 1.86                     | 0.40              |
| 51:B4:23:ILE:H     | 51:B4:23:ILE:HG12  | 1.64                     | 0.40              |
| 52:BI:75:ALA:HB3   | 52:BI:131:THR:HG21 | 2.03                     | 0.40              |
| 1:CA:37:U:O2'      | 1:CA:38:G:H5'      | 2.21                     | 0.40              |
| 1:CA:546:A:H4'     | 1:CA:548:G:O3'     | 2.21                     | 0.40              |
| 1:CA:551:U:H2'     | 1:CA:552:U:H6      | 1.86                     | 0.40              |
| 1:CA:621:A:H2'     | 1:CA:622:A:H8      | 1.82                     | 0.40              |
| 1:CA:812:G:OP1     | 1:CA:812:G:C4'     | 2.70                     | 0.40              |
| 1:CA:1336:C:H4'    | 1:CA:1337:G:O5'    | 2.21                     | 0.40              |
| 3:CD:27:ILE:C      | 3:CD:29:THR:N      | 2.80                     | 0.40              |
| 3:CD:47:LEU:HD11   | 3:CD:51:GLY:C      | 2.47                     | 0.40              |
| 3:CD:77:GLU:C      | 3:CD:79:ALA:H      | 2.29                     | 0.40              |
| 4:CE:61:LYS:HG3    | 4:CE:62:ALA:N      | 2.35                     | 0.40              |
| 5:CF:89:VAL:O      | 5:CF:89:VAL:HG13   | 2.20                     | 0.40              |
| 10:CK:70:ALA:C     | 10:CK:74:LYS:HB2   | 2.46                     | 0.40              |
| 11:CL:20:VAL:HG23  | 11:CL:20:VAL:O     | 2.22                     | 0.40              |
| 12:CM:22:TYR:O     | 12:CM:24:VAL:N     | 2.55                     | 0.40              |
| 13:CN:48:GLN:HG3   | 13:CN:48:GLN:H     | 1.61                     | 0.40              |
| 14:CO:10:ILE:HG21  | 14:CO:30:LEU:HD21  | 2.03                     | 0.40              |
| 16:CQ:57:VAL:HG12  | 16:CQ:78:VAL:HB    | 2.03                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 16:CQ:60:ILE:HB   | 16:CQ:73:THR:O     | 2.21                     | 0.40              |
| 18:CS:28:LYS:HD2  | 18:CS:28:LYS:N     | 2.37                     | 0.40              |
| 19:CT:68:LYS:HB2  | 19:CT:70:LYS:CD    | 2.51                     | 0.40              |
| 20:CB:48:MET:CB   | 20:CB:199:ILE:HG22 | 2.52                     | 0.40              |
| 20:CB:64:GLY:O    | 20:CB:66:ILE:HG12  | 2.22                     | 0.40              |
| 20:CB:69:VAL:CG2  | 20:CB:160:LEU:HD11 | 2.51                     | 0.40              |
| 20:CB:186:VAL:O   | 20:CB:200:PRO:HA   | 2.22                     | 0.40              |
| 22:DA:116:G:H4'   | 36:DO:54:VAL:HG22  | 2.02                     | 0.40              |
| 23:DB:483:A:O2'   | 42:DU:43:LYS:NZ    | 2.55                     | 0.40              |
| 23:DB:769:U:H2'   | 23:DB:770:G:C8     | 2.57                     | 0.40              |
| 23:DB:988:A:H5''  | 45:DY:10:ARG:HD3   | 2.03                     | 0.40              |
| 23:DB:1176:U:O5'  | 23:DB:1176:U:H6    | 2.04                     | 0.40              |
| 23:DB:1275:A:N3   | 23:DB:1275:A:C3'   | 2.79                     | 0.40              |
| 23:DB:1275:A:C8   | 35:DN:16:HIS:HB2   | 2.57                     | 0.40              |
| 23:DB:1300:G:H4'  | 23:DB:1301:A:O5'   | 2.21                     | 0.40              |
| 23:DB:2586:U:H2'  | 23:DB:2587:A:H8    | 1.84                     | 0.40              |
| 55:DB:3475:HOH:O  | 35:DN:4:ARG:HA     | 2.21                     | 0.40              |
| 25:DC:28:PRO:CD   | 25:DC:79:ARG:HE    | 2.34                     | 0.40              |
| 26:DD:18:ASP:O    | 26:DD:20:VAL:N     | 2.54                     | 0.40              |
| 26:DD:95:SER:HB3  | 26:DD:96:ILE:H     | 1.65                     | 0.40              |
| 27:DE:51:GLU:HG2  | 27:DE:52:VAL:HG13  | 2.03                     | 0.40              |
| 29:DG:171:LYS:HZ3 | 29:DG:173:ALA:HA   | 1.86                     | 0.40              |
| 30:DH:122:LEU:HA  | 30:DH:146:VAL:CG2  | 2.49                     | 0.40              |
| 30:DH:127:GLU:H   | 30:DH:127:GLU:CD   | 2.29                     | 0.40              |
| 31:DJ:7:LYS:CE    | 31:DJ:45:THR:HG21  | 2.52                     | 0.40              |
| 31:DJ:7:LYS:O     | 31:DJ:48:VAL:HG21  | 2.20                     | 0.40              |
| 32:DK:2:ILE:N     | 32:DK:2:ILE:HD12   | 2.35                     | 0.40              |
| 32:DK:5:GLN:O     | 32:DK:20:MET:HG3   | 2.21                     | 0.40              |
| 32:DK:113:MET:C   | 32:DK:115:ILE:N    | 2.78                     | 0.40              |
| 33:DL:77:ILE:HD11 | 33:DL:108:ALA:O    | 2.21                     | 0.40              |
| 35:DN:70:THR:HG23 | 35:DN:72:ASP:HB3   | 2.04                     | 0.40              |
| 37:DP:59:THR:HG23 | 37:DP:76:HIS:NE2   | 2.36                     | 0.40              |
| 38:DQ:50:ARG:HH22 | 38:DQ:53:LYS:CE    | 2.34                     | 0.40              |
| 38:DQ:57:ARG:O    | 38:DQ:61:ILE:HG13  | 2.21                     | 0.40              |
| 38:DQ:86:SER:HB3  | 38:DQ:88:GLU:OE2   | 2.21                     | 0.40              |
| 39:DR:74:ILE:HD11 | 39:DR:76:LYS:HE2   | 2.03                     | 0.40              |
| 40:DS:36:LEU:O    | 40:DS:39:THR:HG22  | 2.21                     | 0.40              |
| 41:DT:19:LYS:HA   | 41:DT:19:LYS:HD2   | 1.88                     | 0.40              |
| 41:DT:66:LYS:HB3  | 41:DT:66:LYS:NZ    | 2.35                     | 0.40              |
| 41:DT:70:HIS:CG   | 41:DT:71:GLY:H     | 2.39                     | 0.40              |
| 44:DX:11:VAL:C    | 44:DX:13:GLU:H     | 2.30                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 44:DX:22:LEU:HD23  | 44:DX:22:LEU:HA   | 1.97                     | 0.40              |
| 46:DZ:3:LYS:HG2    | 46:DZ:51:VAL:HG21 | 2.04                     | 0.40              |
| 48:D1:10:LEU:H     | 48:D1:24:LYS:CB   | 2.31                     | 0.40              |
| 50:D3:12:ARG:O     | 50:D3:13:PHE:CB   | 2.69                     | 0.40              |
| 1:AA:137:U:H2'     | 1:AA:138:G:C8     | 2.57                     | 0.40              |
| 1:AA:607:A:H2'     | 1:AA:608:A:H8     | 1.86                     | 0.40              |
| 1:AA:620:C:H1'     | 3:AD:131:ILE:HG21 | 2.03                     | 0.40              |
| 1:AA:1226:C:O2'    | 1:AA:1227:A:P     | 2.79                     | 0.40              |
| 1:AA:1315:U:H3'    | 1:AA:1316:G:C8    | 2.56                     | 0.40              |
| 2:AC:10:ARG:O      | 2:AC:15:LYS:HB2   | 2.20                     | 0.40              |
| 2:AC:155:ARG:CZ    | 2:AC:192:TYR:HB2  | 2.51                     | 0.40              |
| 3:AD:25:ARG:HD3    | 3:AD:26:ALA:N     | 2.30                     | 0.40              |
| 4:AE:19:ARG:HA     | 4:AE:32:PHE:HA    | 2.03                     | 0.40              |
| 8:AI:38:PHE:HD2    | 8:AI:38:PHE:HA    | 1.77                     | 0.40              |
| 9:AJ:92:LEU:H      | 9:AJ:92:LEU:CD2   | 2.29                     | 0.40              |
| 10:AK:35:ASP:HB3   | 10:AK:41:LEU:HD11 | 2.04                     | 0.40              |
| 11:AL:66:ILE:CD1   | 11:AL:73:LEU:HD12 | 2.51                     | 0.40              |
| 17:AR:46:THR:O     | 17:AR:50:TYR:HB2  | 2.21                     | 0.40              |
| 17:AR:64:LEU:C     | 17:AR:66:LEU:N    | 2.78                     | 0.40              |
| 19:AT:40:ALA:O     | 19:AT:41:GLY:C    | 2.63                     | 0.40              |
| 23:BB:539:G:O2'    | 23:BB:540:C:H5'   | 2.22                     | 0.40              |
| 23:BB:711:G:C2'    | 23:BB:712:G:H5'   | 2.51                     | 0.40              |
| 23:BB:1345:C:H5'   | 23:BB:1396:U:H5   | 1.86                     | 0.40              |
| 23:BB:1655:A:H2'   | 23:BB:1656:C:O4'  | 2.22                     | 0.40              |
| 23:BB:1723:G:N7    | 23:BB:1724:G:N7   | 2.70                     | 0.40              |
| 23:BB:1736:U:H2'   | 23:BB:1737:G:O4'  | 2.20                     | 0.40              |
| 23:BB:1801:A:H5'   | 23:BB:2203:U:O2'  | 2.21                     | 0.40              |
| 23:BB:2331:G:H2'   | 23:BB:2332:C:C6   | 2.57                     | 0.40              |
| 23:BB:2617:U:C4    | 23:BB:2618:G:N7   | 2.90                     | 0.40              |
| 24:BV:82:TYR:HB3   | 34:BM:36:VAL:HG12 | 2.04                     | 0.40              |
| 26:BD:165:MET:HE3  | 26:BD:166:GLY:N   | 2.32                     | 0.40              |
| 26:BD:168:GLU:HG2  | 26:BD:169:ARG:N   | 2.37                     | 0.40              |
| 26:BD:175:LEU:HB3  | 26:BD:189:VAL:CG1 | 2.52                     | 0.40              |
| 26:BD:196:ALA:C    | 26:BD:198:GLY:H   | 2.29                     | 0.40              |
| 27:BE:193:VAL:HG11 | 27:BE:201:ALA:HA  | 2.02                     | 0.40              |
| 31:BJ:25:LEU:HG    | 31:BJ:64:VAL:N    | 2.25                     | 0.40              |
| 33:BL:93:ASN:O     | 33:BL:94:THR:HB   | 2.21                     | 0.40              |
| 34:BM:126:ILE:HG13 | 34:BM:127:LYS:N   | 2.25                     | 0.40              |
| 35:BN:116:VAL:HG22 | 35:BN:117:ASP:N   | 2.27                     | 0.40              |
| 36:BO:17:LYS:HG2   | 43:BW:77:LYS:HD2  | 2.02                     | 0.40              |
| 38:BQ:68:ALA:HB2   | 38:BQ:105:PHE:HZ  | 1.87                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:BT:2:ILE:O     | 41:BT:5:GLU:OE1   | 2.39                     | 0.40              |
| 44:BX:6:LEU:C     | 44:BX:8:GLU:H     | 2.29                     | 0.40              |
| 45:BY:18:LYS:HD2  | 45:BY:53:MET:HE1  | 2.02                     | 0.40              |
| 46:BZ:6:HIS:H     | 46:BZ:51:VAL:HG13 | 1.86                     | 0.40              |
| 46:BZ:48:GLN:O    | 46:BZ:51:VAL:HB   | 2.20                     | 0.40              |
| 47:B0:9:ARG:O     | 47:B0:10:SER:HB3  | 2.22                     | 0.40              |
| 47:B0:35:GLU:CG   | 47:B0:36:LYS:H    | 2.34                     | 0.40              |
| 48:B1:8:ILE:HB    | 48:B1:9:LYS:H     | 1.60                     | 0.40              |
| 48:B1:44:GLN:OE1  | 48:B1:46:VAL:HB   | 2.22                     | 0.40              |
| 52:BI:4:VAL:O     | 52:BI:4:VAL:HG13  | 2.21                     | 0.40              |
| 1:CA:258:G:N2     | 1:CA:259:G:H1'    | 2.37                     | 0.40              |
| 1:CA:265:G:H5'    | 16:CQ:65:PRO:O    | 2.20                     | 0.40              |
| 1:CA:279:A:C5'    | 1:CA:280:C:H3'    | 2.48                     | 0.40              |
| 1:CA:415:A:N1     | 1:CA:428:G:O6     | 2.54                     | 0.40              |
| 1:CA:525:C:OP1    | 11:CL:87:LYS:HE2  | 2.21                     | 0.40              |
| 1:CA:1284:C:H3'   | 1:CA:1285:A:H8    | 1.86                     | 0.40              |
| 1:CA:1475:G:H4'   | 23:DB:1689:A:H4'  | 2.03                     | 0.40              |
| 1:CA:1503:A:C8    | 1:CA:1531:A:H1'   | 2.56                     | 0.40              |
| 1:CA:1515:G:O2'   | 1:CA:1516:G:H5'   | 2.21                     | 0.40              |
| 2:CC:127:VAL:CG2  | 2:CC:128:MET:H    | 2.25                     | 0.40              |
| 2:CC:145:ALA:C    | 2:CC:147:GLY:H    | 2.30                     | 0.40              |
| 3:CD:58:GLN:HE21  | 3:CD:58:GLN:CA    | 2.16                     | 0.40              |
| 3:CD:68:GLU:O     | 3:CD:69:ARG:C     | 2.65                     | 0.40              |
| 3:CD:105:GLY:HA3  | 3:CD:158:LEU:HD23 | 2.03                     | 0.40              |
| 5:CF:11:HIS:HB3   | 5:CF:14:GLN:HB2   | 2.02                     | 0.40              |
| 5:CF:59:TYR:HD1   | 5:CF:59:TYR:H     | 1.68                     | 0.40              |
| 9:CJ:36:VAL:O     | 9:CJ:37:ARG:C     | 2.65                     | 0.40              |
| 11:CL:53:ARG:HG2  | 11:CL:63:THR:HG22 | 2.03                     | 0.40              |
| 12:CM:56:ARG:HA   | 12:CM:59:VAL:CG1  | 2.51                     | 0.40              |
| 14:CO:44:GLU:C    | 14:CO:46:LYS:N    | 2.77                     | 0.40              |
| 16:CQ:11:VAL:HG13 | 16:CQ:20:ILE:CG2  | 2.47                     | 0.40              |
| 16:CQ:75:VAL:CG2  | 16:CQ:76:ARG:N    | 2.85                     | 0.40              |
| 19:CT:11:ILE:HG13 | 19:CT:12:GLN:N    | 2.36                     | 0.40              |
| 20:CB:59:ILE:HD12 | 20:CB:59:ILE:C    | 2.46                     | 0.40              |
| 20:CB:130:LYS:C   | 20:CB:132:GLU:N   | 2.80                     | 0.40              |
| 21:CU:32:ARG:HG2  | 21:CU:32:ARG:O    | 2.21                     | 0.40              |
| 22:DA:23:G:C2     | 22:DA:24:G:N1     | 2.90                     | 0.40              |
| 22:DA:25:U:O5'    | 22:DA:26:C:OP1    | 2.40                     | 0.40              |
| 22:DA:115:A:H2'   | 22:DA:116:G:O4'   | 2.22                     | 0.40              |
| 23:DB:44:A:H2'    | 23:DB:45:G:O4'    | 2.22                     | 0.40              |
| 23:DB:239:C:H2'   | 23:DB:240:C:H6    | 1.87                     | 0.40              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:265:A:H2'   | 23:DB:266:G:H1'    | 2.03                     | 0.40              |
| 23:DB:297:G:H2'   | 23:DB:298:G:C8     | 2.56                     | 0.40              |
| 23:DB:562:U:H2'   | 23:DB:572:A:O4'    | 2.21                     | 0.40              |
| 23:DB:649:G:H2'   | 23:DB:650:C:C6     | 2.56                     | 0.40              |
| 23:DB:811:U:H3'   | 33:DL:32:GLY:O     | 2.21                     | 0.40              |
| 23:DB:1050:A:O2'  | 23:DB:1051:G:H5'   | 2.22                     | 0.40              |
| 23:DB:1099:G:N7   | 52:DI:3:LYS:CD     | 2.83                     | 0.40              |
| 23:DB:1266:G:O2'  | 23:DB:1267:U:OP2   | 2.38                     | 0.40              |
| 23:DB:1537:G:C2'  | 23:DB:1538:G:H5'   | 2.51                     | 0.40              |
| 23:DB:1769:U:O2'  | 23:DB:1770:G:H5'   | 2.22                     | 0.40              |
| 23:DB:2379:G:H2'  | 23:DB:2380:C:H6    | 1.87                     | 0.40              |
| 23:DB:2617:U:O2'  | 23:DB:2618:G:H5'   | 2.22                     | 0.40              |
| 23:DB:2759:G:H2'  | 23:DB:2760:C:O4'   | 2.21                     | 0.40              |
| 23:DB:2799:A:H4'  | 23:DB:2800:A:C8    | 2.56                     | 0.40              |
| 24:DV:65:VAL:C    | 24:DV:67:GLY:N     | 2.79                     | 0.40              |
| 25:DC:19:VAL:CG1  | 25:DC:20:ASN:H     | 2.33                     | 0.40              |
| 26:DD:168:GLU:CD  | 26:DD:168:GLU:N    | 2.79                     | 0.40              |
| 27:DE:138:LEU:HB2 | 27:DE:143:LEU:CD1  | 2.51                     | 0.40              |
| 27:DE:198:GLU:HB3 | 27:DE:199:MET:H    | 1.59                     | 0.40              |
| 29:DG:9:VAL:HB    | 29:DG:11:PRO:HD3   | 2.03                     | 0.40              |
| 30:DH:90:LEU:HD22 | 30:DH:122:LEU:HB3  | 2.03                     | 0.40              |
| 32:DK:76:VAL:H    | 37:DP:74:GLN:HB2   | 1.86                     | 0.40              |
| 35:DN:2:ARG:CZ    | 35:DN:4:ARG:NH1    | 2.85                     | 0.40              |
| 35:DN:33:ILE:C    | 35:DN:34:ILE:HD13  | 2.46                     | 0.40              |
| 36:DO:62:LEU:HD12 | 36:DO:62:LEU:H     | 1.87                     | 0.40              |
| 40:DS:86:MET:HG3  | 40:DS:87:PRO:CD    | 2.51                     | 0.40              |
| 41:DT:3:ARG:HB3   | 41:DT:5:GLU:OE1    | 2.21                     | 0.40              |
| 43:DW:33:GLY:C    | 43:DW:66:VAL:HG23  | 2.47                     | 0.40              |
| 43:DW:43:LYS:CD   | 43:DW:76:ARG:HA    | 2.49                     | 0.40              |
| 47:D0:53:VAL:CG1  | 47:D0:54:ILE:N     | 2.85                     | 0.40              |
| 49:D2:4:THR:O     | 49:D2:5:PHE:HB2    | 2.21                     | 0.40              |
| 51:D4:36:ARG:HD2  | 51:D4:37:GLN:O     | 2.22                     | 0.40              |
| 52:DI:78:LEU:HD13 | 52:DI:108:ILE:HG23 | 2.03                     | 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 |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 2   | AC    | 204/233 (88%) | 144 (71%) | 44 (22%) | 16 (8%)  | 1           | 8  |
| 2   | CC    | 204/233 (88%) | 138 (68%) | 46 (22%) | 20 (10%) | 0           | 6  |
| 3   | AD    | 203/206 (98%) | 133 (66%) | 49 (24%) | 21 (10%) | 0           | 6  |
| 3   | CD    | 203/206 (98%) | 137 (68%) | 49 (24%) | 17 (8%)  | 0           | 7  |
| 4   | AE    | 148/167 (89%) | 110 (74%) | 30 (20%) | 8 (5%)   | 1           | 14 |
| 4   | CE    | 148/167 (89%) | 109 (74%) | 30 (20%) | 9 (6%)   | 1           | 12 |
| 5   | AF    | 98/135 (73%)  | 68 (69%)  | 25 (26%) | 5 (5%)   | 1           | 15 |
| 5   | CF    | 98/135 (73%)  | 72 (74%)  | 18 (18%) | 8 (8%)   | 0           | 8  |
| 6   | AG    | 148/179 (83%) | 105 (71%) | 35 (24%) | 8 (5%)   | 1           | 14 |
| 6   | CG    | 150/179 (84%) | 101 (67%) | 37 (25%) | 12 (8%)  | 1           | 8  |
| 7   | AH    | 127/130 (98%) | 108 (85%) | 14 (11%) | 5 (4%)   | 2           | 20 |
| 7   | CH    | 127/130 (98%) | 91 (72%)  | 29 (23%) | 7 (6%)   | 1           | 14 |
| 8   | AI    | 125/130 (96%) | 84 (67%)  | 30 (24%) | 11 (9%)  | 0           | 7  |
| 8   | CI    | 125/130 (96%) | 82 (66%)  | 30 (24%) | 13 (10%) | 0           | 6  |
| 9   | AJ    | 96/103 (93%)  | 65 (68%)  | 20 (21%) | 11 (12%) | 0           | 5  |
| 9   | CJ    | 96/103 (93%)  | 59 (62%)  | 18 (19%) | 19 (20%) | 0           | 1  |
| 10  | AK    | 115/129 (89%) | 75 (65%)  | 32 (28%) | 8 (7%)   | 1           | 10 |
| 10  | CK    | 115/129 (89%) | 76 (66%)  | 30 (26%) | 9 (8%)   | 1           | 8  |
| 11  | AL    | 121/124 (98%) | 73 (60%)  | 35 (29%) | 13 (11%) | 0           | 5  |
| 11  | CL    | 121/124 (98%) | 76 (63%)  | 28 (23%) | 17 (14%) | 0           | 3  |
| 12  | AM    | 112/118 (95%) | 89 (80%)  | 13 (12%) | 10 (9%)  | 0           | 7  |
| 12  | CM    | 111/118 (94%) | 82 (74%)  | 17 (15%) | 12 (11%) | 0           | 5  |
| 13  | AN    | 92/101 (91%)  | 64 (70%)  | 19 (21%) | 9 (10%)  | 0           | 6  |
| 13  | CN    | 92/101 (91%)  | 50 (54%)  | 26 (28%) | 16 (17%) | 0           | 2  |
| 14  | AO    | 86/89 (97%)   | 66 (77%)  | 19 (22%) | 1 (1%)   | 10          | 41 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed      | Favoured  | Allowed   | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|-----------|----------|-------------|----|
| 14  | CO    | 86/89 (97%)   | 69 (80%)  | 15 (17%)  | 2 (2%)   | 5           | 30 |
| 15  | AP    | 80/82 (98%)   | 60 (75%)  | 14 (18%)  | 6 (8%)   | 1           | 9  |
| 15  | CP    | 78/82 (95%)   | 55 (70%)  | 14 (18%)  | 9 (12%)  | 0           | 5  |
| 16  | AQ    | 78/84 (93%)   | 49 (63%)  | 25 (32%)  | 4 (5%)   | 1           | 15 |
| 16  | CQ    | 79/84 (94%)   | 58 (73%)  | 15 (19%)  | 6 (8%)   | 1           | 8  |
| 17  | AR    | 53/75 (71%)   | 31 (58%)  | 16 (30%)  | 6 (11%)  | 0           | 5  |
| 17  | CR    | 53/75 (71%)   | 36 (68%)  | 13 (24%)  | 4 (8%)   | 1           | 9  |
| 18  | AS    | 77/92 (84%)   | 54 (70%)  | 12 (16%)  | 11 (14%) | 0           | 3  |
| 18  | CS    | 78/92 (85%)   | 50 (64%)  | 17 (22%)  | 11 (14%) | 0           | 3  |
| 19  | AT    | 83/87 (95%)   | 68 (82%)  | 12 (14%)  | 3 (4%)   | 2           | 22 |
| 19  | CT    | 83/87 (95%)   | 62 (75%)  | 16 (19%)  | 5 (6%)   | 1           | 12 |
| 20  | AB    | 216/241 (90%) | 148 (68%) | 52 (24%)  | 16 (7%)  | 1           | 9  |
| 20  | CB    | 216/241 (90%) | 149 (69%) | 41 (19%)  | 26 (12%) | 0           | 4  |
| 21  | AU    | 49/71 (69%)   | 23 (47%)  | 12 (24%)  | 14 (29%) | 0           | 0  |
| 21  | CU    | 49/71 (69%)   | 26 (53%)  | 18 (37%)  | 5 (10%)  | 0           | 6  |
| 24  | BV    | 92/94 (98%)   | 61 (66%)  | 24 (26%)  | 7 (8%)   | 1           | 8  |
| 24  | DV    | 92/94 (98%)   | 64 (70%)  | 23 (25%)  | 5 (5%)   | 1           | 14 |
| 25  | BC    | 265/273 (97%) | 94 (36%)  | 95 (36%)  | 76 (29%) | 0           | 0  |
| 25  | DC    | 265/273 (97%) | 97 (37%)  | 101 (38%) | 67 (25%) | 0           | 0  |
| 26  | BD    | 207/209 (99%) | 87 (42%)  | 68 (33%)  | 52 (25%) | 0           | 0  |
| 26  | DD    | 207/209 (99%) | 91 (44%)  | 72 (35%)  | 44 (21%) | 0           | 1  |
| 27  | BE    | 199/201 (99%) | 101 (51%) | 57 (29%)  | 41 (21%) | 0           | 1  |
| 27  | DE    | 199/201 (99%) | 90 (45%)  | 63 (32%)  | 46 (23%) | 0           | 1  |
| 28  | BF    | 176/179 (98%) | 99 (56%)  | 42 (24%)  | 35 (20%) | 0           | 1  |
| 28  | DF    | 176/179 (98%) | 98 (56%)  | 49 (28%)  | 29 (16%) | 0           | 2  |
| 29  | BG    | 174/177 (98%) | 112 (64%) | 41 (24%)  | 21 (12%) | 0           | 4  |
| 29  | DG    | 174/177 (98%) | 108 (62%) | 51 (29%)  | 15 (9%)  | 0           | 7  |
| 30  | BH    | 147/149 (99%) | 83 (56%)  | 49 (33%)  | 15 (10%) | 0           | 6  |
| 30  | DH    | 147/149 (99%) | 83 (56%)  | 46 (31%)  | 18 (12%) | 0           | 4  |
| 31  | BJ    | 138/142 (97%) | 68 (49%)  | 43 (31%)  | 27 (20%) | 0           | 1  |
| 31  | DJ    | 138/142 (97%) | 72 (52%)  | 36 (26%)  | 30 (22%) | 0           | 1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed      | Favoured | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|----------|----------|----------|-------------|----|
| 32  | BK    | 119/123 (97%) | 73 (61%) | 27 (23%) | 19 (16%) | 0           | 2  |
| 32  | DK    | 119/123 (97%) | 70 (59%) | 30 (25%) | 19 (16%) | 0           | 2  |
| 33  | BL    | 142/144 (99%) | 56 (39%) | 47 (33%) | 39 (28%) | 0           | 0  |
| 33  | DL    | 142/144 (99%) | 68 (48%) | 35 (25%) | 39 (28%) | 0           | 0  |
| 34  | BM    | 134/136 (98%) | 64 (48%) | 37 (28%) | 33 (25%) | 0           | 0  |
| 34  | DM    | 134/136 (98%) | 71 (53%) | 43 (32%) | 20 (15%) | 0           | 2  |
| 35  | BN    | 125/127 (98%) | 68 (54%) | 41 (33%) | 16 (13%) | 0           | 4  |
| 35  | DN    | 125/127 (98%) | 86 (69%) | 29 (23%) | 10 (8%)  | 1           | 8  |
| 36  | BO    | 115/117 (98%) | 61 (53%) | 34 (30%) | 20 (17%) | 0           | 2  |
| 36  | DO    | 115/117 (98%) | 62 (54%) | 33 (29%) | 20 (17%) | 0           | 2  |
| 37  | BP    | 112/115 (97%) | 37 (33%) | 38 (34%) | 37 (33%) | 0           | 0  |
| 37  | DP    | 112/115 (97%) | 42 (38%) | 37 (33%) | 33 (30%) | 0           | 0  |
| 38  | BQ    | 115/118 (98%) | 79 (69%) | 23 (20%) | 13 (11%) | 0           | 5  |
| 38  | DQ    | 115/118 (98%) | 78 (68%) | 21 (18%) | 16 (14%) | 0           | 3  |
| 39  | BR    | 101/103 (98%) | 39 (39%) | 38 (38%) | 24 (24%) | 0           | 0  |
| 39  | DR    | 101/103 (98%) | 42 (42%) | 30 (30%) | 29 (29%) | 0           | 0  |
| 40  | BS    | 108/110 (98%) | 58 (54%) | 34 (32%) | 16 (15%) | 0           | 3  |
| 40  | DS    | 108/110 (98%) | 62 (57%) | 26 (24%) | 20 (18%) | 0           | 1  |
| 41  | BT    | 97/100 (97%)  | 38 (39%) | 42 (43%) | 17 (18%) | 0           | 2  |
| 41  | DT    | 97/100 (97%)  | 44 (45%) | 28 (29%) | 25 (26%) | 0           | 0  |
| 42  | BU    | 100/104 (96%) | 36 (36%) | 43 (43%) | 21 (21%) | 0           | 1  |
| 42  | DU    | 100/104 (96%) | 47 (47%) | 34 (34%) | 19 (19%) | 0           | 1  |
| 43  | BW    | 82/85 (96%)   | 35 (43%) | 22 (27%) | 25 (30%) | 0           | 0  |
| 43  | DW    | 82/85 (96%)   | 28 (34%) | 31 (38%) | 23 (28%) | 0           | 0  |
| 44  | BX    | 61/63 (97%)   | 20 (33%) | 30 (49%) | 11 (18%) | 0           | 1  |
| 44  | DX    | 61/63 (97%)   | 37 (61%) | 15 (25%) | 9 (15%)  | 0           | 3  |
| 45  | BY    | 56/59 (95%)   | 29 (52%) | 17 (30%) | 10 (18%) | 0           | 2  |
| 45  | DY    | 56/59 (95%)   | 38 (68%) | 15 (27%) | 3 (5%)   | 1           | 14 |
| 46  | BZ    | 68/70 (97%)   | 32 (47%) | 23 (34%) | 13 (19%) | 0           | 1  |
| 46  | DZ    | 68/70 (97%)   | 36 (53%) | 22 (32%) | 10 (15%) | 0           | 3  |
| 47  | B0    | 54/57 (95%)   | 27 (50%) | 17 (32%) | 10 (18%) | 0           | 1  |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Analysed          | Favoured   | Allowed    | Outliers   | Percentiles |    |
|-----|-------|-------------------|------------|------------|------------|-------------|----|
| 47  | D0    | 54/57 (95%)       | 25 (46%)   | 20 (37%)   | 9 (17%)    | 0           | 2  |
| 48  | B1    | 52/55 (94%)       | 22 (42%)   | 20 (38%)   | 10 (19%)   | 0           | 1  |
| 48  | D1    | 52/55 (94%)       | 21 (40%)   | 18 (35%)   | 13 (25%)   | 0           | 0  |
| 49  | B2    | 44/46 (96%)       | 22 (50%)   | 15 (34%)   | 7 (16%)    | 0           | 2  |
| 49  | D2    | 44/46 (96%)       | 22 (50%)   | 10 (23%)   | 12 (27%)   | 0           | 0  |
| 50  | B3    | 62/65 (95%)       | 26 (42%)   | 28 (45%)   | 8 (13%)    | 0           | 4  |
| 50  | D3    | 62/65 (95%)       | 30 (48%)   | 21 (34%)   | 11 (18%)   | 0           | 2  |
| 51  | B4    | 36/38 (95%)       | 17 (47%)   | 9 (25%)    | 10 (28%)   | 0           | 0  |
| 51  | D4    | 36/38 (95%)       | 13 (36%)   | 10 (28%)   | 13 (36%)   | 0           | 0  |
| 52  | BI    | 139/142 (98%)     | 122 (88%)  | 12 (9%)    | 5 (4%)     | 2           | 22 |
| 52  | DI    | 139/142 (98%)     | 119 (86%)  | 15 (11%)   | 5 (4%)     | 2           | 22 |
| All | All   | 11263/11954 (94%) | 6605 (59%) | 2995 (27%) | 1663 (15%) | 0           | 3  |

All (1663) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AC    | 2   | GLN  |
| 2   | AC    | 81  | GLU  |
| 2   | AC    | 91  | ALA  |
| 3   | AD    | 18  | LEU  |
| 3   | AD    | 25  | ARG  |
| 3   | AD    | 191 | SER  |
| 5   | AF    | 92  | THR  |
| 8   | AI    | 8   | THR  |
| 9   | AJ    | 57  | VAL  |
| 10  | AK    | 56  | LYS  |
| 10  | AK    | 126 | ARG  |
| 11  | AL    | 23  | LEU  |
| 11  | AL    | 72  | ASN  |
| 11  | AL    | 104 | SER  |
| 12  | AM    | 6   | ILE  |
| 12  | AM    | 14  | ALA  |
| 15  | AP    | 79  | ASN  |
| 15  | AP    | 81  | ALA  |
| 20  | AB    | 19  | THR  |
| 20  | AB    | 22  | TRP  |
| 20  | AB    | 163 | ILE  |
| 21  | AU    | 14  | ALA  |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | AU    | 22  | CYS  |
| 25  | BC    | 21  | PRO  |
| 25  | BC    | 22  | GLU  |
| 25  | BC    | 28  | PRO  |
| 25  | BC    | 29  | PHE  |
| 25  | BC    | 31  | PRO  |
| 25  | BC    | 32  | LEU  |
| 25  | BC    | 47  | ARG  |
| 25  | BC    | 63  | ILE  |
| 25  | BC    | 64  | VAL  |
| 25  | BC    | 67  | LYS  |
| 25  | BC    | 68  | ARG  |
| 25  | BC    | 72  | GLY  |
| 25  | BC    | 97  | ASP  |
| 25  | BC    | 103 | ILE  |
| 25  | BC    | 114 | GLN  |
| 25  | BC    | 124 | LYS  |
| 25  | BC    | 135 | PRO  |
| 25  | BC    | 140 | VAL  |
| 25  | BC    | 141 | HIS  |
| 25  | BC    | 149 | LYS  |
| 25  | BC    | 156 | SER  |
| 25  | BC    | 176 | ARG  |
| 25  | BC    | 227 | VAL  |
| 25  | BC    | 246 | PRO  |
| 25  | BC    | 266 | ILE  |
| 26  | BD    | 9   | VAL  |
| 26  | BD    | 14  | ILE  |
| 26  | BD    | 33  | ARG  |
| 26  | BD    | 59  | ARG  |
| 26  | BD    | 84  | LEU  |
| 26  | BD    | 114 | LYS  |
| 26  | BD    | 127 | PHE  |
| 26  | BD    | 128 | ARG  |
| 26  | BD    | 130 | GLN  |
| 26  | BD    | 139 | SER  |
| 26  | BD    | 140 | HIS  |
| 26  | BD    | 141 | ARG  |
| 26  | BD    | 150 | GLN  |
| 26  | BD    | 154 | LYS  |
| 26  | BD    | 155 | VAL  |
| 26  | BD    | 170 | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | BE    | 4   | VAL  |
| 27  | BE    | 44  | ARG  |
| 27  | BE    | 52  | VAL  |
| 27  | BE    | 59  | PRO  |
| 27  | BE    | 84  | THR  |
| 27  | BE    | 117 | ARG  |
| 27  | BE    | 129 | PRO  |
| 27  | BE    | 165 | HIS  |
| 27  | BE    | 196 | VAL  |
| 28  | BF    | 31  | GLU  |
| 28  | BF    | 46  | LYS  |
| 28  | BF    | 66  | ILE  |
| 28  | BF    | 73  | VAL  |
| 28  | BF    | 76  | PHE  |
| 28  | BF    | 131 | VAL  |
| 28  | BF    | 139 | GLU  |
| 28  | BF    | 149 | ARG  |
| 29  | BG    | 6   | ALA  |
| 29  | BG    | 25  | ILE  |
| 29  | BG    | 91  | VAL  |
| 29  | BG    | 151 | ARG  |
| 30  | BH    | 29  | PHE  |
| 30  | BH    | 37  | VAL  |
| 30  | BH    | 38  | PRO  |
| 30  | BH    | 41  | LYS  |
| 31  | BJ    | 4   | PHE  |
| 31  | BJ    | 43  | GLU  |
| 31  | BJ    | 44  | TYR  |
| 31  | BJ    | 64  | VAL  |
| 31  | BJ    | 73  | VAL  |
| 31  | BJ    | 100 | VAL  |
| 31  | BJ    | 101 | ILE  |
| 31  | BJ    | 119 | PHE  |
| 31  | BJ    | 137 | PRO  |
| 32  | BK    | 25  | LEU  |
| 32  | BK    | 35  | VAL  |
| 32  | BK    | 53  | LYS  |
| 32  | BK    | 71  | ARG  |
| 32  | BK    | 72  | PRO  |
| 32  | BK    | 89  | ASN  |
| 32  | BK    | 110 | GLU  |
| 32  | BK    | 120 | PRO  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | BL    | 17  | LYS  |
| 33  | BL    | 56  | PRO  |
| 33  | BL    | 62  | PRO  |
| 33  | BL    | 73  | ILE  |
| 33  | BL    | 84  | LYS  |
| 33  | BL    | 85  | VAL  |
| 33  | BL    | 90  | VAL  |
| 33  | BL    | 91  | ASP  |
| 33  | BL    | 92  | LEU  |
| 33  | BL    | 104 | GLN  |
| 33  | BL    | 118 | THR  |
| 33  | BL    | 119 | PRO  |
| 33  | BL    | 126 | ARG  |
| 33  | BL    | 127 | VAL  |
| 33  | BL    | 141 | LYS  |
| 34  | BM    | 3   | GLN  |
| 34  | BM    | 4   | PRO  |
| 34  | BM    | 14  | LYS  |
| 34  | BM    | 69  | PRO  |
| 34  | BM    | 80  | VAL  |
| 34  | BM    | 81  | ARG  |
| 34  | BM    | 98  | PRO  |
| 34  | BM    | 109 | PRO  |
| 35  | BN    | 3   | HIS  |
| 35  | BN    | 4   | ARG  |
| 35  | BN    | 8   | ARG  |
| 35  | BN    | 37  | THR  |
| 35  | BN    | 89  | SER  |
| 35  | BN    | 107 | ASN  |
| 35  | BN    | 113 | ILE  |
| 35  | BN    | 116 | VAL  |
| 36  | BO    | 37  | ALA  |
| 36  | BO    | 42  | PRO  |
| 36  | BO    | 54  | VAL  |
| 36  | BO    | 63  | LYS  |
| 37  | BP    | 23  | ASP  |
| 37  | BP    | 24  | THR  |
| 37  | BP    | 49  | ILE  |
| 37  | BP    | 55  | HIS  |
| 37  | BP    | 60  | VAL  |
| 37  | BP    | 82  | SER  |
| 37  | BP    | 83  | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | BP    | 85  | VAL  |
| 37  | BP    | 90  | ALA  |
| 37  | BP    | 91  | VAL  |
| 37  | BP    | 94  | ALA  |
| 37  | BP    | 111 | GLU  |
| 38  | BQ    | 34  | ALA  |
| 38  | BQ    | 89  | ILE  |
| 38  | BQ    | 92  | LYS  |
| 39  | BR    | 15  | SER  |
| 39  | BR    | 24  | LYS  |
| 39  | BR    | 47  | VAL  |
| 39  | BR    | 59  | ILE  |
| 39  | BR    | 74  | ILE  |
| 39  | BR    | 101 | ILE  |
| 40  | BS    | 6   | LYS  |
| 40  | BS    | 103 | ILE  |
| 41  | BT    | 32  | LEU  |
| 41  | BT    | 63  | VAL  |
| 42  | BU    | 4   | ILE  |
| 42  | BU    | 21  | ARG  |
| 42  | BU    | 63  | ALA  |
| 42  | BU    | 92  | VAL  |
| 43  | BW    | 11  | ASN  |
| 43  | BW    | 18  | LYS  |
| 43  | BW    | 44  | PHE  |
| 43  | BW    | 53  | GLY  |
| 43  | BW    | 66  | VAL  |
| 43  | BW    | 67  | LYS  |
| 43  | BW    | 75  | ASN  |
| 43  | BW    | 81  | ILE  |
| 44  | BX    | 24  | GLU  |
| 44  | BX    | 33  | ALA  |
| 44  | BX    | 46  | VAL  |
| 45  | BY    | 9   | THR  |
| 45  | BY    | 51  | SER  |
| 46  | BZ    | 4   | ASP  |
| 46  | BZ    | 7   | PRO  |
| 46  | BZ    | 8   | LYS  |
| 46  | BZ    | 26  | SER  |
| 46  | BZ    | 60  | PHE  |
| 47  | B0    | 29  | VAL  |
| 47  | B0    | 35  | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | B1    | 45  | HIS  |
| 48  | B1    | 46  | VAL  |
| 49  | B2    | 4   | THR  |
| 49  | B2    | 43  | THR  |
| 49  | B2    | 44  | VAL  |
| 50  | B3    | 16  | THR  |
| 50  | B3    | 23  | HIS  |
| 50  | B3    | 57  | VAL  |
| 50  | B3    | 60  | CYS  |
| 51  | B4    | 5   | ALA  |
| 51  | B4    | 17  | VAL  |
| 51  | B4    | 24  | ARG  |
| 51  | B4    | 29  | ALA  |
| 51  | B4    | 35  | GLN  |
| 52  | BI    | 18  | ASN  |
| 2   | CC    | 54  | ILE  |
| 3   | CD    | 24  | VAL  |
| 3   | CD    | 49  | ASP  |
| 3   | CD    | 121 | ALA  |
| 4   | CE    | 23  | THR  |
| 5   | CF    | 98  | GLU  |
| 6   | CG    | 3   | ARG  |
| 6   | CG    | 62  | GLU  |
| 7   | CH    | 66  | GLN  |
| 7   | CH    | 82  | LEU  |
| 9   | CJ    | 34  | ALA  |
| 9   | CJ    | 57  | VAL  |
| 9   | CJ    | 61  | ALA  |
| 9   | CJ    | 67  | ILE  |
| 11  | CL    | 10  | PRO  |
| 11  | CL    | 32  | VAL  |
| 11  | CL    | 33  | CYS  |
| 11  | CL    | 43  | LYS  |
| 11  | CL    | 88  | ASP  |
| 11  | CL    | 101 | LEU  |
| 11  | CL    | 111 | GLN  |
| 12  | CM    | 22  | TYR  |
| 12  | CM    | 105 | ALA  |
| 13  | CN    | 29  | ILE  |
| 13  | CN    | 50  | LEU  |
| 14  | CO    | 73  | ASP  |
| 15  | CP    | 28  | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | CS    | 29  | PRO  |
| 18  | CS    | 62  | THR  |
| 19  | CT    | 3   | ILE  |
| 19  | CT    | 4   | LYS  |
| 20  | CB    | 22  | TRP  |
| 20  | CB    | 73  | ARG  |
| 20  | CB    | 188 | THR  |
| 20  | CB    | 206 | ILE  |
| 20  | CB    | 208 | ALA  |
| 25  | DC    | 28  | PRO  |
| 25  | DC    | 29  | PHE  |
| 25  | DC    | 31  | PRO  |
| 25  | DC    | 32  | LEU  |
| 25  | DC    | 47  | ARG  |
| 25  | DC    | 63  | ILE  |
| 25  | DC    | 87  | SER  |
| 25  | DC    | 88  | ALA  |
| 25  | DC    | 97  | ASP  |
| 25  | DC    | 121 | ALA  |
| 25  | DC    | 125 | PRO  |
| 25  | DC    | 135 | PRO  |
| 25  | DC    | 149 | LYS  |
| 25  | DC    | 157 | ALA  |
| 25  | DC    | 163 | ILE  |
| 25  | DC    | 164 | VAL  |
| 25  | DC    | 176 | ARG  |
| 25  | DC    | 194 | VAL  |
| 25  | DC    | 200 | MET  |
| 25  | DC    | 246 | PRO  |
| 25  | DC    | 259 | ASN  |
| 25  | DC    | 266 | ILE  |
| 26  | DD    | 9   | VAL  |
| 26  | DD    | 34  | VAL  |
| 26  | DD    | 39  | ASP  |
| 26  | DD    | 45  | TYR  |
| 26  | DD    | 55  | LYS  |
| 26  | DD    | 82  | PHE  |
| 26  | DD    | 84  | LEU  |
| 26  | DD    | 85  | ALA  |
| 26  | DD    | 129 | THR  |
| 26  | DD    | 140 | HIS  |
| 26  | DD    | 152 | PRO  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | DD    | 155 | VAL  |
| 26  | DD    | 157 | LYS  |
| 26  | DD    | 160 | LYS  |
| 27  | DE    | 17  | THR  |
| 27  | DE    | 45  | ALA  |
| 27  | DE    | 86  | ALA  |
| 27  | DE    | 91  | ASP  |
| 27  | DE    | 147 | LEU  |
| 27  | DE    | 162 | ARG  |
| 28  | DF    | 46  | LYS  |
| 28  | DF    | 73  | VAL  |
| 28  | DF    | 84  | ILE  |
| 28  | DF    | 133 | GLU  |
| 28  | DF    | 173 | ASP  |
| 29  | DG    | 2   | ARG  |
| 29  | DG    | 4   | ALA  |
| 29  | DG    | 6   | ALA  |
| 29  | DG    | 101 | VAL  |
| 30  | DH    | 11  | ASN  |
| 30  | DH    | 38  | PRO  |
| 30  | DH    | 121 | VAL  |
| 31  | DJ    | 4   | PHE  |
| 31  | DJ    | 11  | VAL  |
| 31  | DJ    | 43  | GLU  |
| 31  | DJ    | 44  | TYR  |
| 31  | DJ    | 64  | VAL  |
| 31  | DJ    | 78  | THR  |
| 31  | DJ    | 81  | ILE  |
| 31  | DJ    | 124 | VAL  |
| 32  | DK    | 71  | ARG  |
| 32  | DK    | 72  | PRO  |
| 32  | DK    | 113 | MET  |
| 32  | DK    | 120 | PRO  |
| 33  | DL    | 7   | SER  |
| 33  | DL    | 8   | PRO  |
| 33  | DL    | 17  | LYS  |
| 33  | DL    | 38  | GLN  |
| 33  | DL    | 51  | GLU  |
| 33  | DL    | 54  | GLN  |
| 33  | DL    | 72  | ALA  |
| 33  | DL    | 92  | LEU  |
| 33  | DL    | 111 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | DL    | 119 | PRO  |
| 33  | DL    | 126 | ARG  |
| 33  | DL    | 127 | VAL  |
| 33  | DL    | 142 | ILE  |
| 34  | DM    | 5   | LYS  |
| 34  | DM    | 16  | ARG  |
| 34  | DM    | 17  | ASN  |
| 34  | DM    | 65  | ILE  |
| 34  | DM    | 71  | LYS  |
| 34  | DM    | 72  | PRO  |
| 34  | DM    | 84  | LYS  |
| 34  | DM    | 86  | LYS  |
| 34  | DM    | 101 | VAL  |
| 34  | DM    | 106 | ASP  |
| 34  | DM    | 109 | PRO  |
| 35  | DN    | 91  | ALA  |
| 36  | DO    | 23  | ALA  |
| 36  | DO    | 27  | VAL  |
| 36  | DO    | 54  | VAL  |
| 36  | DO    | 63  | LYS  |
| 36  | DO    | 90  | VAL  |
| 37  | DP    | 17  | PRO  |
| 37  | DP    | 23  | ASP  |
| 37  | DP    | 24  | THR  |
| 37  | DP    | 41  | ALA  |
| 37  | DP    | 60  | VAL  |
| 37  | DP    | 71  | ARG  |
| 37  | DP    | 72  | VAL  |
| 37  | DP    | 76  | HIS  |
| 37  | DP    | 77  | SER  |
| 37  | DP    | 79  | VAL  |
| 37  | DP    | 80  | VAL  |
| 37  | DP    | 82  | SER  |
| 37  | DP    | 105 | LYS  |
| 37  | DP    | 110 | LYS  |
| 37  | DP    | 111 | GLU  |
| 38  | DQ    | 73  | ILE  |
| 38  | DQ    | 89  | ILE  |
| 38  | DQ    | 93  | ILE  |
| 39  | DR    | 22  | LEU  |
| 39  | DR    | 27  | ILE  |
| 39  | DR    | 73  | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | DR    | 75  | VAL  |
| 39  | DR    | 89  | HIS  |
| 39  | DR    | 90  | ARG  |
| 39  | DR    | 97  | LYS  |
| 40  | DS    | 60  | HIS  |
| 40  | DS    | 103 | ILE  |
| 41  | DT    | 27  | SER  |
| 41  | DT    | 57  | VAL  |
| 41  | DT    | 62  | VAL  |
| 41  | DT    | 95  | PHE  |
| 42  | DU    | 30  | SER  |
| 42  | DU    | 63  | ALA  |
| 42  | DU    | 66  | VAL  |
| 42  | DU    | 75  | ALA  |
| 43  | DW    | 30  | VAL  |
| 43  | DW    | 34  | SER  |
| 43  | DW    | 44  | PHE  |
| 43  | DW    | 57  | THR  |
| 43  | DW    | 58  | LEU  |
| 43  | DW    | 66  | VAL  |
| 46  | DZ    | 21  | VAL  |
| 46  | DZ    | 28  | VAL  |
| 46  | DZ    | 31  | ASP  |
| 46  | DZ    | 40  | CYS  |
| 47  | D0    | 31  | LYS  |
| 47  | D0    | 45  | ASP  |
| 48  | D1    | 14  | ALA  |
| 48  | D1    | 23  | THR  |
| 48  | D1    | 46  | VAL  |
| 49  | D2    | 44  | VAL  |
| 50  | D3    | 30  | HIS  |
| 51  | D4    | 3   | VAL  |
| 51  | D4    | 17  | VAL  |
| 51  | D4    | 19  | ARG  |
| 51  | D4    | 24  | ARG  |
| 51  | D4    | 26  | ILE  |
| 51  | D4    | 27  | CYS  |
| 52  | DI    | 18  | ASN  |
| 2   | AC    | 100 | ILE  |
| 2   | AC    | 153 | SER  |
| 3   | AD    | 31  | CYS  |
| 3   | AD    | 107 | GLY  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | AD    | 152 | SER  |
| 3   | AD    | 172 | VAL  |
| 3   | AD    | 192 | ALA  |
| 4   | AE    | 20  | VAL  |
| 4   | AE    | 76  | ASN  |
| 4   | AE    | 107 | GLY  |
| 5   | AF    | 62  | MET  |
| 6   | AG    | 18  | GLY  |
| 6   | AG    | 129 | ASN  |
| 8   | AI    | 43  | ALA  |
| 8   | AI    | 57  | VAL  |
| 8   | AI    | 108 | ARG  |
| 9   | AJ    | 74  | VAL  |
| 9   | AJ    | 75  | ASP  |
| 10  | AK    | 53  | GLY  |
| 11  | AL    | 10  | PRO  |
| 11  | AL    | 84  | GLY  |
| 12  | AM    | 3   | ILE  |
| 12  | AM    | 7   | ASN  |
| 12  | AM    | 66  | GLY  |
| 12  | AM    | 104 | ASN  |
| 13  | AN    | 51  | PRO  |
| 13  | AN    | 52  | ARG  |
| 13  | AN    | 61  | ASN  |
| 13  | AN    | 94  | GLY  |
| 15  | AP    | 29  | ASN  |
| 16  | AQ    | 6   | THR  |
| 16  | AQ    | 34  | GLY  |
| 16  | AQ    | 69  | THR  |
| 17  | AR    | 20  | ILE  |
| 17  | AR    | 22  | TYR  |
| 17  | AR    | 71  | ASP  |
| 18  | AS    | 5   | LYS  |
| 19  | AT    | 3   | ILE  |
| 19  | AT    | 85  | LEU  |
| 21  | AU    | 32  | ARG  |
| 21  | AU    | 33  | ARG  |
| 21  | AU    | 52  | VAL  |
| 24  | BV    | 45  | ASP  |
| 25  | BC    | 4   | LYS  |
| 25  | BC    | 14  | HIS  |
| 25  | BC    | 48  | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | BC    | 51  | ARG  |
| 25  | BC    | 90  | ILE  |
| 25  | BC    | 107 | LYS  |
| 25  | BC    | 111 | ALA  |
| 25  | BC    | 143 | VAL  |
| 25  | BC    | 157 | ALA  |
| 25  | BC    | 163 | ILE  |
| 25  | BC    | 194 | VAL  |
| 25  | BC    | 208 | GLY  |
| 25  | BC    | 209 | ALA  |
| 25  | BC    | 226 | PRO  |
| 26  | BD    | 2   | ILE  |
| 26  | BD    | 16  | THR  |
| 26  | BD    | 27  | ILE  |
| 26  | BD    | 30  | GLU  |
| 26  | BD    | 42  | ASN  |
| 26  | BD    | 101 | PHE  |
| 26  | BD    | 104 | VAL  |
| 26  | BD    | 125 | TRP  |
| 26  | BD    | 129 | THR  |
| 26  | BD    | 169 | ARG  |
| 26  | BD    | 202 | ILE  |
| 26  | BD    | 205 | PRO  |
| 26  | BD    | 206 | ALA  |
| 26  | BD    | 207 | VAL  |
| 27  | BE    | 23  | PHE  |
| 27  | BE    | 26  | ALA  |
| 27  | BE    | 37  | ALA  |
| 27  | BE    | 47  | LYS  |
| 27  | BE    | 49  | ARG  |
| 27  | BE    | 54  | GLY  |
| 27  | BE    | 61  | ARG  |
| 27  | BE    | 68  | ALA  |
| 27  | BE    | 86  | ALA  |
| 27  | BE    | 90  | GLN  |
| 27  | BE    | 104 | ALA  |
| 27  | BE    | 120 | VAL  |
| 27  | BE    | 128 | ALA  |
| 27  | BE    | 146 | VAL  |
| 27  | BE    | 148 | ILE  |
| 27  | BE    | 169 | VAL  |
| 27  | BE    | 171 | ASP  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | BF    | 14  | LYS  |
| 28  | BF    | 114 | ARG  |
| 28  | BF    | 136 | ILE  |
| 28  | BF    | 153 | ILE  |
| 28  | BF    | 162 | ASP  |
| 28  | BF    | 176 | PHE  |
| 29  | BG    | 2   | ARG  |
| 29  | BG    | 32  | LEU  |
| 29  | BG    | 42  | VAL  |
| 29  | BG    | 47  | ASN  |
| 29  | BG    | 173 | ALA  |
| 30  | BH    | 8   | LYS  |
| 30  | BH    | 44  | ILE  |
| 30  | BH    | 65  | ALA  |
| 30  | BH    | 127 | GLU  |
| 30  | BH    | 134 | VAL  |
| 31  | BJ    | 6   | ALA  |
| 31  | BJ    | 18  | VAL  |
| 31  | BJ    | 79  | GLY  |
| 31  | BJ    | 81  | ILE  |
| 31  | BJ    | 84  | ILE  |
| 31  | BJ    | 138 | GLN  |
| 32  | BK    | 17  | ARG  |
| 32  | BK    | 92  | GLU  |
| 33  | BL    | 15  | ALA  |
| 33  | BL    | 29  | LYS  |
| 33  | BL    | 31  | GLY  |
| 33  | BL    | 53  | GLY  |
| 33  | BL    | 94  | THR  |
| 33  | BL    | 95  | LEU  |
| 33  | BL    | 117 | THR  |
| 33  | BL    | 120 | VAL  |
| 33  | BL    | 143 | GLU  |
| 34  | BM    | 7   | THR  |
| 34  | BM    | 36  | VAL  |
| 34  | BM    | 58  | LYS  |
| 34  | BM    | 70  | ASP  |
| 34  | BM    | 86  | LYS  |
| 34  | BM    | 87  | GLY  |
| 34  | BM    | 104 | GLU  |
| 34  | BM    | 132 | THR  |
| 35  | BN    | 11  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | BN    | 94  | TYR  |
| 35  | BN    | 104 | ALA  |
| 35  | BN    | 114 | GLU  |
| 36  | BO    | 9   | ARG  |
| 36  | BO    | 21  | LEU  |
| 36  | BO    | 28  | VAL  |
| 36  | BO    | 38  | GLN  |
| 36  | BO    | 47  | VAL  |
| 36  | BO    | 49  | VAL  |
| 36  | BO    | 95  | SER  |
| 36  | BO    | 115 | LEU  |
| 37  | BP    | 29  | VAL  |
| 37  | BP    | 30  | TRP  |
| 37  | BP    | 41  | ALA  |
| 37  | BP    | 56  | SER  |
| 37  | BP    | 59  | THR  |
| 37  | BP    | 62  | LYS  |
| 37  | BP    | 72  | VAL  |
| 37  | BP    | 76  | HIS  |
| 37  | BP    | 80  | VAL  |
| 37  | BP    | 81  | ASP  |
| 37  | BP    | 97  | TYR  |
| 37  | BP    | 102 | ARG  |
| 37  | BP    | 105 | LYS  |
| 37  | BP    | 110 | LYS  |
| 37  | BP    | 112 | ARG  |
| 38  | BQ    | 21  | LYS  |
| 38  | BQ    | 23  | TYR  |
| 38  | BQ    | 33  | VAL  |
| 38  | BQ    | 78  | PHE  |
| 38  | BQ    | 91  | ARG  |
| 38  | BQ    | 93  | ILE  |
| 39  | BR    | 17  | GLY  |
| 39  | BR    | 25  | LEU  |
| 39  | BR    | 29  | THR  |
| 39  | BR    | 37  | GLU  |
| 39  | BR    | 87  | GLN  |
| 39  | BR    | 98  | ILE  |
| 39  | BR    | 100 | GLY  |
| 40  | BS    | 3   | THR  |
| 40  | BS    | 5   | ALA  |
| 40  | BS    | 29  | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | BS    | 67  | ASP  |
| 40  | BS    | 96  | ILE  |
| 41  | BT    | 4   | GLU  |
| 41  | BT    | 6   | ARG  |
| 41  | BT    | 14  | PRO  |
| 41  | BT    | 15  | HIS  |
| 41  | BT    | 30  | ILE  |
| 41  | BT    | 34  | VAL  |
| 41  | BT    | 67  | VAL  |
| 41  | BT    | 74  | ILE  |
| 41  | BT    | 81  | LYS  |
| 41  | BT    | 85  | VAL  |
| 42  | BU    | 14  | THR  |
| 42  | BU    | 24  | VAL  |
| 42  | BU    | 35  | VAL  |
| 42  | BU    | 45  | GLN  |
| 42  | BU    | 54  | PRO  |
| 42  | BU    | 60  | LYS  |
| 42  | BU    | 64  | ILE  |
| 42  | BU    | 71  | ILE  |
| 42  | BU    | 77  | GLY  |
| 43  | BW    | 23  | LYS  |
| 43  | BW    | 38  | ARG  |
| 43  | BW    | 40  | ARG  |
| 43  | BW    | 50  | VAL  |
| 43  | BW    | 63  | ASP  |
| 43  | BW    | 72  | GLY  |
| 43  | BW    | 77  | LYS  |
| 44  | BX    | 9   | LYS  |
| 44  | BX    | 16  | THR  |
| 44  | BX    | 36  | GLN  |
| 44  | BX    | 40  | SER  |
| 45  | BY    | 3   | THR  |
| 45  | BY    | 12  | ALA  |
| 46  | BZ    | 9   | TYR  |
| 46  | BZ    | 39  | LYS  |
| 46  | BZ    | 40  | CYS  |
| 46  | BZ    | 58  | ASP  |
| 47  | B0    | 41  | HIS  |
| 47  | B0    | 49  | ARG  |
| 49  | B2    | 36  | ALA  |
| 50  | B3    | 15  | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | B4    | 20  | ASP  |
| 51  | B4    | 22  | VAL  |
| 2   | CC    | 25  | THR  |
| 2   | CC    | 63  | ILE  |
| 2   | CC    | 65  | VAL  |
| 2   | CC    | 95  | GLY  |
| 2   | CC    | 128 | MET  |
| 2   | CC    | 153 | SER  |
| 3   | CD    | 14  | GLU  |
| 3   | CD    | 47  | LEU  |
| 3   | CD    | 120 | LYS  |
| 3   | CD    | 169 | TRP  |
| 4   | CE    | 15  | ILE  |
| 4   | CE    | 17  | VAL  |
| 4   | CE    | 107 | GLY  |
| 5   | CF    | 89  | VAL  |
| 6   | CG    | 16  | LYS  |
| 6   | CG    | 113 | LYS  |
| 6   | CG    | 130 | LYS  |
| 7   | CH    | 69  | ALA  |
| 7   | CH    | 122 | GLY  |
| 8   | CI    | 24  | ASN  |
| 8   | CI    | 57  | VAL  |
| 9   | CJ    | 33  | GLY  |
| 9   | CJ    | 37  | ARG  |
| 9   | CJ    | 60  | ASP  |
| 9   | CJ    | 74  | VAL  |
| 9   | CJ    | 77  | VAL  |
| 9   | CJ    | 94  | ALA  |
| 10  | CK    | 14  | GLN  |
| 10  | CK    | 17  | ASP  |
| 11  | CL    | 13  | ARG  |
| 11  | CL    | 97  | VAL  |
| 11  | CL    | 104 | SER  |
| 11  | CL    | 117 | GLY  |
| 11  | CL    | 121 | PRO  |
| 12  | CM    | 3   | ILE  |
| 12  | CM    | 7   | ASN  |
| 12  | CM    | 23  | GLY  |
| 13  | CN    | 21  | ALA  |
| 13  | CN    | 51  | PRO  |
| 14  | CO    | 3   | SER  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | CP    | 46  | LYS  |
| 15  | CP    | 79  | ASN  |
| 16  | CQ    | 28  | VAL  |
| 16  | CQ    | 47  | ASP  |
| 16  | CQ    | 56  | ASP  |
| 16  | CQ    | 69  | THR  |
| 17  | CR    | 21  | ASP  |
| 18  | CS    | 27  | LYS  |
| 18  | CS    | 69  | LYS  |
| 20  | CB    | 18  | GLN  |
| 20  | CB    | 19  | THR  |
| 20  | CB    | 72  | LYS  |
| 20  | CB    | 97  | GLY  |
| 20  | CB    | 124 | THR  |
| 20  | CB    | 193 | ASP  |
| 21  | CU    | 22  | CYS  |
| 24  | DV    | 14  | LYS  |
| 24  | DV    | 45  | ASP  |
| 24  | DV    | 70  | ILE  |
| 25  | DC    | 21  | PRO  |
| 25  | DC    | 22  | GLU  |
| 25  | DC    | 39  | SER  |
| 25  | DC    | 43  | ASN  |
| 25  | DC    | 52  | HIS  |
| 25  | DC    | 53  | ILE  |
| 25  | DC    | 65  | ASP  |
| 25  | DC    | 70  | LYS  |
| 25  | DC    | 90  | ILE  |
| 25  | DC    | 93  | VAL  |
| 25  | DC    | 106 | PRO  |
| 25  | DC    | 156 | SER  |
| 25  | DC    | 173 | LEU  |
| 25  | DC    | 199 | HIS  |
| 25  | DC    | 201 | LEU  |
| 25  | DC    | 210 | ALA  |
| 25  | DC    | 227 | VAL  |
| 25  | DC    | 252 | LYS  |
| 26  | DD    | 43  | ASP  |
| 26  | DD    | 73  | VAL  |
| 26  | DD    | 77  | ARG  |
| 26  | DD    | 89  | GLU  |
| 26  | DD    | 95  | SER  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | DD    | 145 | SER  |
| 26  | DD    | 168 | GLU  |
| 26  | DD    | 184 | ARG  |
| 26  | DD    | 185 | ASN  |
| 26  | DD    | 187 | LEU  |
| 26  | DD    | 193 | VAL  |
| 26  | DD    | 197 | THR  |
| 26  | DD    | 205 | PRO  |
| 26  | DD    | 206 | ALA  |
| 27  | DE    | 4   | VAL  |
| 27  | DE    | 7   | ASP  |
| 27  | DE    | 13  | THR  |
| 27  | DE    | 43  | THR  |
| 27  | DE    | 48  | THR  |
| 27  | DE    | 49  | ARG  |
| 27  | DE    | 54  | GLY  |
| 27  | DE    | 59  | PRO  |
| 27  | DE    | 84  | THR  |
| 27  | DE    | 85  | PHE  |
| 27  | DE    | 110 | SER  |
| 27  | DE    | 115 | GLN  |
| 27  | DE    | 126 | VAL  |
| 27  | DE    | 148 | ILE  |
| 27  | DE    | 149 | ILE  |
| 27  | DE    | 153 | LEU  |
| 27  | DE    | 166 | LYS  |
| 27  | DE    | 168 | ASP  |
| 27  | DE    | 195 | GLN  |
| 28  | DF    | 20  | ASN  |
| 28  | DF    | 49  | LEU  |
| 28  | DF    | 66  | ILE  |
| 28  | DF    | 80  | GLN  |
| 28  | DF    | 83  | PRO  |
| 28  | DF    | 109 | ARG  |
| 28  | DF    | 136 | ILE  |
| 28  | DF    | 149 | ARG  |
| 28  | DF    | 150 | GLY  |
| 28  | DF    | 174 | PHE  |
| 29  | DG    | 5   | LYS  |
| 29  | DG    | 37  | ASN  |
| 30  | DH    | 10  | ALA  |
| 30  | DH    | 25  | TYR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | DH    | 30  | LEU  |
| 30  | DH    | 82  | SER  |
| 30  | DH    | 91  | PHE  |
| 31  | DJ    | 50  | THR  |
| 31  | DJ    | 65  | THR  |
| 31  | DJ    | 128 | ASN  |
| 31  | DJ    | 129 | GLU  |
| 31  | DJ    | 131 | ASN  |
| 31  | DJ    | 135 | GLN  |
| 32  | DK    | 3   | GLN  |
| 32  | DK    | 10  | VAL  |
| 32  | DK    | 18  | ARG  |
| 32  | DK    | 83  | ALA  |
| 33  | DL    | 15  | ALA  |
| 33  | DL    | 20  | GLY  |
| 33  | DL    | 27  | LEU  |
| 33  | DL    | 40  | SER  |
| 33  | DL    | 64  | PHE  |
| 33  | DL    | 108 | ALA  |
| 33  | DL    | 109 | LYS  |
| 33  | DL    | 110 | VAL  |
| 34  | DM    | 80  | VAL  |
| 34  | DM    | 102 | LEU  |
| 35  | DN    | 100 | CYS  |
| 35  | DN    | 116 | VAL  |
| 36  | DO    | 22  | GLY  |
| 36  | DO    | 65  | THR  |
| 36  | DO    | 84  | GLU  |
| 36  | DO    | 96  | GLY  |
| 36  | DO    | 99  | TYR  |
| 36  | DO    | 101 | GLY  |
| 37  | DP    | 27  | VAL  |
| 37  | DP    | 49  | ILE  |
| 37  | DP    | 69  | VAL  |
| 37  | DP    | 75  | THR  |
| 37  | DP    | 83  | ILE  |
| 37  | DP    | 91  | VAL  |
| 38  | DQ    | 5   | ARG  |
| 38  | DQ    | 30  | VAL  |
| 38  | DQ    | 31  | TYR  |
| 38  | DQ    | 85  | ALA  |
| 38  | DQ    | 88  | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | DR    | 4   | VAL  |
| 39  | DR    | 5   | PHE  |
| 39  | DR    | 11  | GLN  |
| 39  | DR    | 59  | ILE  |
| 39  | DR    | 81  | LYS  |
| 39  | DR    | 82  | HIS  |
| 39  | DR    | 93  | PHE  |
| 40  | DS    | 4   | ILE  |
| 40  | DS    | 12  | SER  |
| 40  | DS    | 26  | GLY  |
| 40  | DS    | 41  | LYS  |
| 40  | DS    | 64  | ALA  |
| 40  | DS    | 69  | LEU  |
| 40  | DS    | 87  | PRO  |
| 41  | DT    | 7   | LEU  |
| 41  | DT    | 15  | HIS  |
| 41  | DT    | 31  | VAL  |
| 41  | DT    | 36  | LYS  |
| 41  | DT    | 52  | GLU  |
| 41  | DT    | 63  | VAL  |
| 41  | DT    | 71  | GLY  |
| 41  | DT    | 85  | VAL  |
| 42  | DU    | 4   | ILE  |
| 42  | DU    | 9   | GLU  |
| 42  | DU    | 24  | VAL  |
| 42  | DU    | 28  | LEU  |
| 42  | DU    | 42  | LYS  |
| 42  | DU    | 93  | ARG  |
| 43  | DW    | 4   | LYS  |
| 43  | DW    | 10  | ARG  |
| 43  | DW    | 18  | LYS  |
| 43  | DW    | 45  | HIS  |
| 43  | DW    | 62  | ALA  |
| 43  | DW    | 75  | ASN  |
| 43  | DW    | 77  | LYS  |
| 44  | DX    | 20  | ASN  |
| 45  | DY    | 12  | ALA  |
| 46  | DZ    | 3   | LYS  |
| 46  | DZ    | 10  | GLU  |
| 47  | D0    | 35  | GLU  |
| 47  | D0    | 47  | TYR  |
| 48  | D1    | 30  | PRO  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | D1    | 38  | PHE  |
| 48  | D1    | 47  | ILE  |
| 48  | D1    | 50  | GLU  |
| 49  | D2    | 5   | PHE  |
| 49  | D2    | 18  | PHE  |
| 49  | D2    | 25  | LYS  |
| 50  | D3    | 5   | THR  |
| 50  | D3    | 26  | ALA  |
| 51  | D4    | 10  | LEU  |
| 2   | AC    | 25  | THR  |
| 2   | AC    | 83  | VAL  |
| 2   | AC    | 136 | ALA  |
| 2   | AC    | 180 | ASP  |
| 3   | AD    | 28  | ASP  |
| 3   | AD    | 148 | ALA  |
| 3   | AD    | 151 | GLN  |
| 4   | AE    | 43  | GLY  |
| 5   | AF    | 65  | GLU  |
| 6   | AG    | 75  | LYS  |
| 7   | AH    | 46  | GLU  |
| 7   | AH    | 65  | PHE  |
| 9   | AJ    | 61  | ALA  |
| 9   | AJ    | 62  | ARG  |
| 9   | AJ    | 92  | LEU  |
| 9   | AJ    | 93  | ALA  |
| 10  | AK    | 77  | GLY  |
| 10  | AK    | 125 | LYS  |
| 11  | AL    | 13  | ARG  |
| 11  | AL    | 15  | VAL  |
| 11  | AL    | 47  | ALA  |
| 11  | AL    | 120 | ARG  |
| 12  | AM    | 22  | TYR  |
| 12  | AM    | 98  | GLY  |
| 13  | AN    | 2   | LYS  |
| 13  | AN    | 80  | ARG  |
| 17  | AR    | 32  | ILE  |
| 18  | AS    | 3   | SER  |
| 20  | AB    | 18  | GLN  |
| 20  | AB    | 20  | ARG  |
| 20  | AB    | 27  | LYS  |
| 20  | AB    | 76  | SER  |
| 20  | AB    | 88  | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | AB    | 186 | VAL  |
| 21  | AU    | 24  | LYS  |
| 21  | AU    | 35  | GLU  |
| 21  | AU    | 40  | PRO  |
| 24  | BV    | 54  | ALA  |
| 24  | BV    | 64  | VAL  |
| 24  | BV    | 71  | LYS  |
| 25  | BC    | 34  | GLU  |
| 25  | BC    | 41  | GLY  |
| 25  | BC    | 52  | HIS  |
| 25  | BC    | 53  | ILE  |
| 25  | BC    | 58  | LYS  |
| 25  | BC    | 59  | GLN  |
| 25  | BC    | 65  | ASP  |
| 25  | BC    | 66  | PHE  |
| 25  | BC    | 91  | ALA  |
| 25  | BC    | 93  | VAL  |
| 25  | BC    | 108 | GLY  |
| 25  | BC    | 125 | PRO  |
| 25  | BC    | 231 | HIS  |
| 25  | BC    | 239 | PHE  |
| 25  | BC    | 251 | THR  |
| 25  | BC    | 255 | LYS  |
| 25  | BC    | 259 | ASN  |
| 26  | BD    | 18  | ASP  |
| 26  | BD    | 21  | SER  |
| 26  | BD    | 23  | PRO  |
| 26  | BD    | 105 | LYS  |
| 26  | BD    | 189 | VAL  |
| 27  | BE    | 11  | ALA  |
| 27  | BE    | 24  | ASN  |
| 27  | BE    | 62  | GLN  |
| 27  | BE    | 93  | SER  |
| 27  | BE    | 191 | ASP  |
| 28  | BF    | 19  | PHE  |
| 28  | BF    | 34  | THR  |
| 28  | BF    | 67  | THR  |
| 28  | BF    | 75  | GLY  |
| 28  | BF    | 81  | GLY  |
| 28  | BF    | 88  | VAL  |
| 28  | BF    | 173 | ASP  |
| 29  | BG    | 127 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | BH    | 125 | THR  |
| 31  | BJ    | 50  | THR  |
| 31  | BJ    | 74  | TYR  |
| 31  | BJ    | 83  | GLY  |
| 31  | BJ    | 85  | LYS  |
| 32  | BK    | 46  | ALA  |
| 32  | BK    | 112 | PHE  |
| 33  | BL    | 22  | GLY  |
| 33  | BL    | 27  | LEU  |
| 33  | BL    | 38  | GLN  |
| 33  | BL    | 48  | ARG  |
| 33  | BL    | 57  | LEU  |
| 34  | BM    | 35  | ALA  |
| 34  | BM    | 59  | ARG  |
| 34  | BM    | 77  | PRO  |
| 34  | BM    | 105 | MET  |
| 34  | BM    | 127 | LYS  |
| 35  | BN    | 6   | SER  |
| 35  | BN    | 102 | PHE  |
| 36  | BO    | 32  | PRO  |
| 36  | BO    | 52  | SER  |
| 36  | BO    | 68  | LYS  |
| 37  | BP    | 17  | PRO  |
| 37  | BP    | 48  | ALA  |
| 37  | BP    | 52  | ARG  |
| 37  | BP    | 71  | ARG  |
| 37  | BP    | 78  | PRO  |
| 38  | BQ    | 73  | ILE  |
| 39  | BR    | 18  | GLN  |
| 39  | BR    | 42  | ALA  |
| 39  | BR    | 45  | GLU  |
| 39  | BR    | 73  | LYS  |
| 39  | BR    | 76  | LYS  |
| 39  | BR    | 77  | PHE  |
| 40  | BS    | 13  | SER  |
| 40  | BS    | 69  | LEU  |
| 41  | BT    | 13  | ALA  |
| 41  | BT    | 61  | LEU  |
| 42  | BU    | 18  | LYS  |
| 42  | BU    | 39  | ASN  |
| 42  | BU    | 67  | SER  |
| 42  | BU    | 72  | PHE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | BU    | 96  | LYS  |
| 43  | BW    | 6   | GLY  |
| 43  | BW    | 49  | ASN  |
| 43  | BW    | 62  | ALA  |
| 43  | BW    | 65  | LYS  |
| 43  | BW    | 68  | PHE  |
| 44  | BX    | 4   | LYS  |
| 44  | BX    | 28  | LEU  |
| 45  | BY    | 14  | GLY  |
| 45  | BY    | 16  | LEU  |
| 45  | BY    | 42  | ALA  |
| 47  | B0    | 4   | GLN  |
| 48  | B1    | 8   | ILE  |
| 48  | B1    | 35  | LEU  |
| 48  | B1    | 43  | ARG  |
| 51  | B4    | 3   | VAL  |
| 51  | B4    | 10  | LEU  |
| 52  | BI    | 14  | ALA  |
| 52  | BI    | 23  | VAL  |
| 2   | CC    | 3   | LYS  |
| 2   | CC    | 145 | ALA  |
| 2   | CC    | 167 | TYR  |
| 5   | CF    | 85  | ILE  |
| 5   | CF    | 95  | ALA  |
| 6   | CG    | 55  | LYS  |
| 7   | CH    | 30  | LYS  |
| 7   | CH    | 53  | ASP  |
| 8   | CI    | 34  | LEU  |
| 8   | CI    | 55  | ASP  |
| 8   | CI    | 106 | ASP  |
| 9   | CJ    | 68  | ARG  |
| 9   | CJ    | 93  | ALA  |
| 9   | CJ    | 100 | ILE  |
| 10  | CK    | 52  | ARG  |
| 10  | CK    | 53  | GLY  |
| 10  | CK    | 88  | PRO  |
| 10  | CK    | 108 | ASN  |
| 11  | CL    | 24  | GLU  |
| 11  | CL    | 73  | LEU  |
| 12  | CM    | 62  | PHE  |
| 12  | CM    | 65  | GLU  |
| 13  | CN    | 33  | VAL  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | CN    | 42  | ASN  |
| 13  | CN    | 43  | ALA  |
| 13  | CN    | 52  | ARG  |
| 13  | CN    | 69  | PRO  |
| 13  | CN    | 70  | HIS  |
| 15  | CP    | 47  | GLU  |
| 18  | CS    | 8   | PRO  |
| 18  | CS    | 34  | SER  |
| 18  | CS    | 63  | ASP  |
| 19  | CT    | 68  | LYS  |
| 20  | CB    | 43  | GLU  |
| 20  | CB    | 44  | LYS  |
| 20  | CB    | 94  | ARG  |
| 20  | CB    | 95  | TRP  |
| 20  | CB    | 114 | LYS  |
| 20  | CB    | 128 | LEU  |
| 20  | CB    | 204 | ASP  |
| 21  | CU    | 23  | GLU  |
| 25  | DC    | 66  | PHE  |
| 25  | DC    | 115 | ILE  |
| 25  | DC    | 172 | THR  |
| 25  | DC    | 184 | GLU  |
| 25  | DC    | 243 | PRO  |
| 25  | DC    | 265 | PHE  |
| 26  | DD    | 47  | ALA  |
| 26  | DD    | 139 | SER  |
| 26  | DD    | 141 | ARG  |
| 26  | DD    | 147 | GLY  |
| 26  | DD    | 174 | SER  |
| 27  | DE    | 30  | GLN  |
| 27  | DE    | 38  | GLY  |
| 27  | DE    | 67  | ARG  |
| 27  | DE    | 90  | GLN  |
| 27  | DE    | 139 | LYS  |
| 27  | DE    | 172 | ALA  |
| 27  | DE    | 190 | ALA  |
| 28  | DF    | 42  | ALA  |
| 28  | DF    | 43  | ILE  |
| 28  | DF    | 88  | VAL  |
| 28  | DF    | 104 | THR  |
| 28  | DF    | 134 | GLN  |
| 28  | DF    | 138 | PRO  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | DF    | 176 | PHE  |
| 29  | DG    | 11  | PRO  |
| 29  | DG    | 45  | ALA  |
| 29  | DG    | 60  | GLY  |
| 29  | DG    | 173 | ALA  |
| 30  | DH    | 31  | VAL  |
| 30  | DH    | 37  | VAL  |
| 30  | DH    | 86  | ASP  |
| 30  | DH    | 92  | GLY  |
| 31  | DJ    | 8   | PRO  |
| 31  | DJ    | 41  | LYS  |
| 31  | DJ    | 53  | TYR  |
| 31  | DJ    | 58  | ASN  |
| 31  | DJ    | 75  | TYR  |
| 31  | DJ    | 77  | HIS  |
| 31  | DJ    | 85  | LYS  |
| 31  | DJ    | 137 | PRO  |
| 32  | DK    | 12  | ASP  |
| 32  | DK    | 17  | ARG  |
| 33  | DL    | 14  | LYS  |
| 33  | DL    | 44  | GLY  |
| 33  | DL    | 45  | GLY  |
| 33  | DL    | 52  | GLY  |
| 33  | DL    | 55  | MET  |
| 33  | DL    | 116 | VAL  |
| 33  | DL    | 141 | LYS  |
| 34  | DM    | 4   | PRO  |
| 34  | DM    | 127 | LYS  |
| 34  | DM    | 128 | THR  |
| 35  | DN    | 32  | GLU  |
| 36  | DO    | 34  | HIS  |
| 36  | DO    | 38  | GLN  |
| 36  | DO    | 87  | ILE  |
| 37  | DP    | 39  | LEU  |
| 37  | DP    | 97  | TYR  |
| 37  | DP    | 112 | ARG  |
| 38  | DQ    | 53  | LYS  |
| 38  | DQ    | 86  | SER  |
| 39  | DR    | 3   | ALA  |
| 39  | DR    | 10  | LYS  |
| 39  | DR    | 42  | ALA  |
| 39  | DR    | 64  | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | DR    | 86  | GLN  |
| 40  | DS    | 9   | HIS  |
| 40  | DS    | 99  | ARG  |
| 41  | DT    | 16  | VAL  |
| 41  | DT    | 39  | THR  |
| 41  | DT    | 68  | LYS  |
| 41  | DT    | 96  | VAL  |
| 42  | DU    | 62  | ALA  |
| 42  | DU    | 64  | ILE  |
| 42  | DU    | 99  | SER  |
| 43  | DW    | 5   | ALA  |
| 43  | DW    | 9   | THR  |
| 43  | DW    | 65  | LYS  |
| 44  | DX    | 28  | LEU  |
| 44  | DX    | 31  | GLN  |
| 44  | DX    | 35  | GLY  |
| 44  | DX    | 52  | ARG  |
| 45  | DY    | 37  | ARG  |
| 46  | DZ    | 26  | SER  |
| 47  | D0    | 36  | LYS  |
| 47  | D0    | 43  | THR  |
| 48  | D1    | 32  | LYS  |
| 49  | D2    | 7   | PRO  |
| 49  | D2    | 8   | SER  |
| 50  | D3    | 10  | ALA  |
| 50  | D3    | 47  | ALA  |
| 51  | D4    | 11  | CYS  |
| 51  | D4    | 31  | PRO  |
| 52  | DI    | 23  | VAL  |
| 2   | AC    | 19  | SER  |
| 2   | AC    | 54  | ILE  |
| 2   | AC    | 65  | VAL  |
| 3   | AD    | 7   | LYS  |
| 3   | AD    | 27  | ILE  |
| 3   | AD    | 29  | THR  |
| 3   | AD    | 143 | SER  |
| 4   | AE    | 34  | ALA  |
| 4   | AE    | 128 | GLY  |
| 5   | AF    | 64  | VAL  |
| 5   | AF    | 94  | HIS  |
| 6   | AG    | 84  | TYR  |
| 8   | AI    | 44  | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | AI    | 55  | ASP  |
| 8   | AI    | 67  | LYS  |
| 8   | AI    | 127 | SER  |
| 9   | AJ    | 36  | VAL  |
| 9   | AJ    | 56  | HIS  |
| 9   | AJ    | 95  | GLY  |
| 11  | AL    | 14  | LYS  |
| 11  | AL    | 122 | LYS  |
| 13  | AN    | 21  | ALA  |
| 15  | AP    | 27  | ALA  |
| 15  | AP    | 42  | ILE  |
| 15  | AP    | 54  | LEU  |
| 18  | AS    | 8   | PRO  |
| 18  | AS    | 15  | LEU  |
| 18  | AS    | 39  | ILE  |
| 19  | AT    | 59  | ARG  |
| 20  | AB    | 41  | ASN  |
| 20  | AB    | 150 | ILE  |
| 20  | AB    | 200 | PRO  |
| 20  | AB    | 205 | ALA  |
| 21  | AU    | 6   | ARG  |
| 21  | AU    | 36  | PHE  |
| 21  | AU    | 37  | TYR  |
| 25  | BC    | 50  | THR  |
| 25  | BC    | 61  | TYR  |
| 25  | BC    | 151 | GLY  |
| 25  | BC    | 165 | ALA  |
| 25  | BC    | 236 | GLY  |
| 25  | BC    | 257 | ARG  |
| 25  | BC    | 258 | SER  |
| 25  | BC    | 265 | PHE  |
| 26  | BD    | 47  | ALA  |
| 26  | BD    | 87  | GLY  |
| 26  | BD    | 90  | PHE  |
| 26  | BD    | 145 | SER  |
| 26  | BD    | 185 | ASN  |
| 26  | BD    | 190 | LYS  |
| 26  | BD    | 193 | VAL  |
| 27  | BE    | 39  | ALA  |
| 27  | BE    | 53  | THR  |
| 27  | BE    | 106 | LYS  |
| 28  | BF    | 7   | TYR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | BF    | 45  | ASP  |
| 28  | BF    | 74  | ALA  |
| 28  | BF    | 172 | PHE  |
| 29  | BG    | 48  | THR  |
| 29  | BG    | 155 | PRO  |
| 29  | BG    | 174 | LYS  |
| 30  | BH    | 20  | ASN  |
| 31  | BJ    | 25  | LEU  |
| 31  | BJ    | 36  | LEU  |
| 31  | BJ    | 97  | PRO  |
| 31  | BJ    | 127 | GLY  |
| 32  | BK    | 6   | THR  |
| 32  | BK    | 121 | GLU  |
| 33  | BL    | 42  | SER  |
| 33  | BL    | 54  | GLN  |
| 33  | BL    | 82  | LEU  |
| 33  | BL    | 109 | LYS  |
| 34  | BM    | 10  | ARG  |
| 34  | BM    | 28  | PHE  |
| 34  | BM    | 133 | LYS  |
| 36  | BO    | 36  | TYR  |
| 36  | BO    | 87  | ILE  |
| 36  | BO    | 90  | VAL  |
| 37  | BP    | 77  | SER  |
| 39  | BR    | 27  | ILE  |
| 39  | BR    | 95  | ASP  |
| 40  | BS    | 11  | ARG  |
| 40  | BS    | 99  | ARG  |
| 41  | BT    | 5   | GLU  |
| 42  | BU    | 3   | LYS  |
| 42  | BU    | 59  | GLU  |
| 43  | BW    | 32  | ALA  |
| 44  | BX    | 7   | ARG  |
| 45  | BY    | 15  | ARG  |
| 45  | BY    | 17  | PRO  |
| 46  | BZ    | 23  | LYS  |
| 47  | B0    | 5   | ASN  |
| 48  | B1    | 5   | ARG  |
| 48  | B1    | 16  | THR  |
| 48  | B1    | 38  | PHE  |
| 48  | B1    | 47  | ILE  |
| 49  | B2    | 42  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | B4    | 7   | VAL  |
| 52  | BI    | 49  | GLU  |
| 52  | BI    | 64  | ARG  |
| 2   | CC    | 50  | SER  |
| 2   | CC    | 59  | PRO  |
| 2   | CC    | 60  | ALA  |
| 2   | CC    | 110 | LEU  |
| 2   | CC    | 144 | GLY  |
| 3   | CD    | 22  | SER  |
| 3   | CD    | 26  | ALA  |
| 3   | CD    | 119 | HIS  |
| 3   | CD    | 166 | LYS  |
| 4   | CE    | 87  | VAL  |
| 4   | CE    | 146 | MET  |
| 6   | CG    | 66  | GLU  |
| 6   | CG    | 78  | ARG  |
| 6   | CG    | 128 | GLU  |
| 6   | CG    | 129 | ASN  |
| 7   | CH    | 94  | VAL  |
| 8   | CI    | 58  | GLU  |
| 8   | CI    | 90  | ASP  |
| 9   | CJ    | 56  | HIS  |
| 9   | CJ    | 75  | ASP  |
| 11  | CL    | 23  | LEU  |
| 12  | CM    | 97  | ARG  |
| 12  | CM    | 102 | LYS  |
| 12  | CM    | 104 | ASN  |
| 13  | CN    | 62  | ARG  |
| 13  | CN    | 65  | GLN  |
| 15  | CP    | 27  | ALA  |
| 18  | CS    | 5   | LYS  |
| 18  | CS    | 22  | VAL  |
| 18  | CS    | 61  | VAL  |
| 18  | CS    | 77  | ARG  |
| 19  | CT    | 67  | HIS  |
| 20  | CB    | 15  | PHE  |
| 20  | CB    | 86  | CYS  |
| 20  | CB    | 126 | ASP  |
| 21  | CU    | 12  | ASP  |
| 24  | DV    | 16  | ALA  |
| 24  | DV    | 71  | LYS  |
| 25  | DC    | 12  | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | DC    | 103 | ILE  |
| 25  | DC    | 113 | ASP  |
| 25  | DC    | 124 | LYS  |
| 25  | DC    | 152 | GLN  |
| 25  | DC    | 226 | PRO  |
| 25  | DC    | 239 | PHE  |
| 26  | DD    | 87  | GLY  |
| 26  | DD    | 173 | GLN  |
| 27  | DE    | 50  | ALA  |
| 27  | DE    | 72  | SER  |
| 27  | DE    | 111 | GLU  |
| 28  | DF    | 34  | THR  |
| 28  | DF    | 36  | ASN  |
| 28  | DF    | 67  | THR  |
| 28  | DF    | 70  | ARG  |
| 29  | DG    | 36  | LEU  |
| 30  | DH    | 114 | GLU  |
| 31  | DJ    | 23  | LYS  |
| 31  | DJ    | 60  | ASP  |
| 31  | DJ    | 134 | ALA  |
| 32  | DK    | 29  | HIS  |
| 32  | DK    | 46  | ALA  |
| 32  | DK    | 84  | CYS  |
| 32  | DK    | 86  | LEU  |
| 32  | DK    | 89  | ASN  |
| 33  | DL    | 5   | THR  |
| 33  | DL    | 60  | ARG  |
| 33  | DL    | 82  | LEU  |
| 33  | DL    | 118 | THR  |
| 34  | DM    | 107 | GLY  |
| 35  | DN    | 99  | LYS  |
| 35  | DN    | 102 | PHE  |
| 35  | DN    | 113 | ILE  |
| 36  | DO    | 2   | ASP  |
| 37  | DP    | 15  | ASP  |
| 37  | DP    | 29  | VAL  |
| 37  | DP    | 33  | GLU  |
| 37  | DP    | 62  | LYS  |
| 37  | DP    | 73  | PHE  |
| 37  | DP    | 90  | ALA  |
| 38  | DQ    | 4   | LYS  |
| 38  | DQ    | 9   | ALA  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | DR    | 71  | LYS  |
| 39  | DR    | 87  | GLN  |
| 39  | DR    | 98  | ILE  |
| 40  | DS    | 8   | ARG  |
| 40  | DS    | 13  | SER  |
| 40  | DS    | 23  | LEU  |
| 40  | DS    | 27  | LYS  |
| 40  | DS    | 80  | PRO  |
| 41  | DT    | 32  | LEU  |
| 41  | DT    | 67  | VAL  |
| 41  | DT    | 79  | ASP  |
| 42  | DU    | 25  | LYS  |
| 42  | DU    | 58  | VAL  |
| 42  | DU    | 94  | PHE  |
| 43  | DW    | 16  | GLU  |
| 43  | DW    | 22  | VAL  |
| 43  | DW    | 61  | LYS  |
| 43  | DW    | 63  | ASP  |
| 43  | DW    | 76  | ARG  |
| 44  | DX    | 36  | GLN  |
| 45  | DY    | 51  | SER  |
| 46  | DZ    | 32  | LEU  |
| 46  | DZ    | 35  | ASP  |
| 47  | D0    | 20  | ALA  |
| 47  | D0    | 51  | ARG  |
| 48  | D1    | 5   | ARG  |
| 48  | D1    | 43  | ARG  |
| 48  | D1    | 51  | ALA  |
| 49  | D2    | 17  | GLY  |
| 49  | D2    | 22  | MET  |
| 51  | D4    | 9   | LYS  |
| 52  | DI    | 14  | ALA  |
| 2   | AC    | 14  | VAL  |
| 2   | AC    | 59  | PRO  |
| 2   | AC    | 145 | ALA  |
| 2   | AC    | 186 | SER  |
| 3   | AD    | 6   | PRO  |
| 3   | AD    | 43  | ARG  |
| 3   | AD    | 177 | MET  |
| 6   | AG    | 57  | GLU  |
| 6   | AG    | 137 | ARG  |
| 10  | AK    | 106 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | AK    | 127 | ARG  |
| 13  | AN    | 14  | ALA  |
| 17  | AR    | 47  | ARG  |
| 18  | AS    | 4   | LEU  |
| 18  | AS    | 27  | LYS  |
| 18  | AS    | 66  | VAL  |
| 20  | AB    | 87  | ASP  |
| 20  | AB    | 121 | GLN  |
| 21  | AU    | 13  | VAL  |
| 21  | AU    | 26  | GLY  |
| 24  | BV    | 70  | ILE  |
| 24  | BV    | 93  | ARG  |
| 25  | BC    | 30  | ALA  |
| 25  | BC    | 40  | GLY  |
| 25  | BC    | 112 | GLY  |
| 25  | BC    | 115 | ILE  |
| 25  | BC    | 196 | ASN  |
| 25  | BC    | 217 | PRO  |
| 25  | BC    | 230 | PRO  |
| 26  | BD    | 52  | THR  |
| 26  | BD    | 162 | ALA  |
| 26  | BD    | 174 | SER  |
| 28  | BF    | 10  | GLU  |
| 28  | BF    | 22  | ASN  |
| 28  | BF    | 77  | LYS  |
| 28  | BF    | 87  | LYS  |
| 28  | BF    | 122 | ASP  |
| 29  | BG    | 11  | PRO  |
| 29  | BG    | 43  | LYS  |
| 29  | BG    | 159 | LYS  |
| 31  | BJ    | 46  | PRO  |
| 31  | BJ    | 53  | TYR  |
| 31  | BJ    | 66  | GLY  |
| 32  | BK    | 3   | GLN  |
| 32  | BK    | 4   | GLU  |
| 32  | BK    | 85  | VAL  |
| 33  | BL    | 114 | GLY  |
| 33  | BL    | 125 | LEU  |
| 33  | BL    | 128 | THR  |
| 34  | BM    | 29  | GLY  |
| 34  | BM    | 30  | SER  |
| 34  | BM    | 125 | PRO  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | BN    | 73  | ASN  |
| 36  | BO    | 31  | THR  |
| 37  | BP    | 39  | LEU  |
| 38  | BQ    | 20  | ALA  |
| 38  | BQ    | 26  | ALA  |
| 39  | BR    | 72  | VAL  |
| 40  | BS    | 9   | HIS  |
| 40  | BS    | 57  | ASN  |
| 40  | BS    | 64  | ALA  |
| 40  | BS    | 71  | VAL  |
| 41  | BT    | 39  | THR  |
| 41  | BT    | 88  | LYS  |
| 43  | BW    | 5   | ALA  |
| 43  | BW    | 31  | LEU  |
| 45  | BY    | 10  | ARG  |
| 46  | BZ    | 5   | ILE  |
| 47  | B0    | 53  | VAL  |
| 48  | B1    | 21  | THR  |
| 49  | B2    | 6   | GLN  |
| 49  | B2    | 17  | GLY  |
| 50  | B3    | 24  | LYS  |
| 50  | B3    | 31  | ILE  |
| 2   | CC    | 100 | ILE  |
| 2   | CC    | 129 | PHE  |
| 3   | CD    | 191 | SER  |
| 3   | CD    | 203 | TYR  |
| 3   | CD    | 204 | SER  |
| 5   | CF    | 53  | LYS  |
| 5   | CF    | 68  | GLN  |
| 8   | CI    | 8   | THR  |
| 8   | CI    | 9   | GLY  |
| 8   | CI    | 121 | ARG  |
| 9   | CJ    | 36  | VAL  |
| 9   | CJ    | 86  | ALA  |
| 10  | CK    | 49  | SER  |
| 12  | CM    | 21  | ILE  |
| 13  | CN    | 31  | SER  |
| 13  | CN    | 73  | LEU  |
| 13  | CN    | 74  | ARG  |
| 15  | CP    | 44  | SER  |
| 15  | CP    | 55  | ASP  |
| 15  | CP    | 69  | ASP  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | CR    | 63  | TYR  |
| 20  | CB    | 211 | LEU  |
| 21  | CU    | 39  | LYS  |
| 25  | DC    | 50  | THR  |
| 25  | DC    | 58  | LYS  |
| 25  | DC    | 137 | GLY  |
| 25  | DC    | 175 | LEU  |
| 26  | DD    | 2   | ILE  |
| 26  | DD    | 49  | GLN  |
| 26  | DD    | 149 | ASN  |
| 27  | DE    | 18  | THR  |
| 27  | DE    | 46  | GLN  |
| 27  | DE    | 89  | PRO  |
| 27  | DE    | 157 | LEU  |
| 27  | DE    | 188 | MET  |
| 27  | DE    | 192 | ALA  |
| 28  | DF    | 10  | GLU  |
| 28  | DF    | 153 | ILE  |
| 29  | DG    | 44  | HIS  |
| 29  | DG    | 151 | ARG  |
| 29  | DG    | 164 | ALA  |
| 30  | DH    | 66  | ASN  |
| 31  | DJ    | 111 | LYS  |
| 31  | DJ    | 125 | TYR  |
| 31  | DJ    | 139 | VAL  |
| 32  | DK    | 14  | SER  |
| 32  | DK    | 26  | GLY  |
| 32  | DK    | 85  | VAL  |
| 33  | DL    | 74  | THR  |
| 34  | DM    | 77  | PRO  |
| 34  | DM    | 82  | MET  |
| 35  | DN    | 41  | ALA  |
| 35  | DN    | 107 | ASN  |
| 36  | DO    | 18  | LEU  |
| 36  | DO    | 103 | VAL  |
| 37  | DP    | 59  | THR  |
| 37  | DP    | 106 | ALA  |
| 38  | DQ    | 78  | PHE  |
| 38  | DQ    | 87  | VAL  |
| 39  | DR    | 37  | GLU  |
| 39  | DR    | 84  | ARG  |
| 40  | DS    | 22  | ASP  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | DS    | 92  | ARG  |
| 41  | DT    | 60  | THR  |
| 41  | DT    | 66  | LYS  |
| 41  | DT    | 86  | THR  |
| 42  | DU    | 57  | ILE  |
| 43  | DW    | 55  | ASP  |
| 44  | DX    | 51  | ALA  |
| 44  | DX    | 61  | ALA  |
| 46  | DZ    | 19  | GLY  |
| 48  | D1    | 21  | THR  |
| 48  | D1    | 29  | LYS  |
| 49  | D2    | 14  | ARG  |
| 49  | D2    | 15  | SER  |
| 49  | D2    | 45  | SER  |
| 50  | D3    | 13  | PHE  |
| 50  | D3    | 29  | ARG  |
| 50  | D3    | 33  | THR  |
| 51  | D4    | 8   | LYS  |
| 52  | DI    | 5   | GLN  |
| 4   | AE    | 25  | LYS  |
| 6   | AG    | 6   | ILE  |
| 6   | AG    | 86  | VAL  |
| 7   | AH    | 82  | LEU  |
| 10  | AK    | 91  | GLY  |
| 12  | AM    | 65  | GLU  |
| 13  | AN    | 33  | VAL  |
| 16  | AQ    | 28  | VAL  |
| 18  | AS    | 36  | ARG  |
| 18  | AS    | 52  | ASN  |
| 18  | AS    | 67  | GLY  |
| 21  | AU    | 23  | GLU  |
| 25  | BC    | 164 | VAL  |
| 25  | BC    | 224 | MET  |
| 26  | BD    | 19  | GLY  |
| 26  | BD    | 99  | GLU  |
| 26  | BD    | 180 | VAL  |
| 27  | BE    | 75  | SER  |
| 27  | BE    | 145 | ASP  |
| 27  | BE    | 186 | VAL  |
| 28  | BF    | 83  | PRO  |
| 28  | BF    | 175 | PRO  |
| 29  | BG    | 84  | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | BH    | 108 | VAL  |
| 31  | BJ    | 121 | LYS  |
| 32  | BK    | 49  | ARG  |
| 34  | BM    | 21  | ALA  |
| 34  | BM    | 26  | VAL  |
| 34  | BM    | 97  | GLN  |
| 35  | BN    | 115 | LEU  |
| 37  | BP    | 26  | GLU  |
| 39  | BR    | 7   | SER  |
| 39  | BR    | 12  | HIS  |
| 42  | BU    | 56  | GLY  |
| 43  | BW    | 42  | THR  |
| 46  | BZ    | 32  | LEU  |
| 46  | BZ    | 66  | ILE  |
| 47  | B0    | 34  | GLY  |
| 50  | B3    | 26  | ALA  |
| 2   | CC    | 127 | VAL  |
| 3   | CD    | 35  | GLN  |
| 3   | CD    | 37  | PRO  |
| 4   | CE    | 20  | VAL  |
| 4   | CE    | 78  | GLY  |
| 5   | CF    | 84  | VAL  |
| 5   | CF    | 99  | ALA  |
| 6   | CG    | 99  | ALA  |
| 8   | CI    | 23  | GLY  |
| 8   | CI    | 71  | ILE  |
| 9   | CJ    | 32  | THR  |
| 9   | CJ    | 62  | ARG  |
| 11  | CL    | 99  | GLY  |
| 11  | CL    | 103 | CYS  |
| 13  | CN    | 3   | GLN  |
| 15  | CP    | 54  | LEU  |
| 17  | CR    | 36  | GLY  |
| 19  | CT    | 44  | ALA  |
| 20  | CB    | 20  | ARG  |
| 20  | CB    | 205 | ALA  |
| 25  | DC    | 60  | ALA  |
| 25  | DC    | 208 | GLY  |
| 25  | DC    | 217 | PRO  |
| 25  | DC    | 224 | MET  |
| 25  | DC    | 244 | VAL  |
| 26  | DD    | 29  | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | DD    | 48  | ILE  |
| 26  | DD    | 53  | GLY  |
| 27  | DE    | 56  | GLY  |
| 27  | DE    | 66  | GLY  |
| 27  | DE    | 167 | VAL  |
| 31  | DJ    | 46  | PRO  |
| 31  | DJ    | 67  | ASN  |
| 33  | DL    | 9   | ALA  |
| 33  | DL    | 49  | GLY  |
| 35  | DN    | 123 | GLU  |
| 37  | DP    | 26  | GLU  |
| 39  | DR    | 54  | VAL  |
| 39  | DR    | 63  | VAL  |
| 39  | DR    | 102 | SER  |
| 40  | DS    | 3   | THR  |
| 40  | DS    | 42  | LYS  |
| 41  | DT    | 76  | ARG  |
| 41  | DT    | 92  | ASN  |
| 42  | DU    | 65  | GLN  |
| 43  | DW    | 52  | CYS  |
| 44  | DX    | 8   | GLU  |
| 50  | D3    | 49  | VAL  |
| 51  | D4    | 28  | SER  |
| 3   | AD    | 175 | GLY  |
| 11  | AL    | 121 | PRO  |
| 14  | AO    | 26  | VAL  |
| 20  | AB    | 24  | PRO  |
| 26  | BD    | 96  | ILE  |
| 27  | BE    | 82  | GLY  |
| 29  | BG    | 7   | PRO  |
| 33  | BL    | 11  | GLY  |
| 33  | BL    | 102 | GLY  |
| 40  | BS    | 4   | ILE  |
| 43  | BW    | 35  | ILE  |
| 47  | B0    | 46  | GLY  |
| 6   | CG    | 18  | GLY  |
| 21  | CU    | 13  | VAL  |
| 26  | DD    | 76  | GLY  |
| 27  | DE    | 58  | LYS  |
| 30  | DH    | 85  | GLY  |
| 32  | DK    | 103 | VAL  |
| 33  | DL    | 32  | GLY  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | DM    | 85  | GLY  |
| 36  | DO    | 28  | VAL  |
| 38  | DQ    | 72  | GLY  |
| 39  | DR    | 33  | VAL  |
| 39  | DR    | 47  | VAL  |
| 4   | AE    | 26  | GLY  |
| 17  | AR    | 43  | ILE  |
| 25  | BC    | 16  | VAL  |
| 25  | BC    | 214 | GLY  |
| 26  | BD    | 73  | VAL  |
| 26  | BD    | 203 | VAL  |
| 28  | BF    | 148 | VAL  |
| 29  | BG    | 110 | HIS  |
| 30  | BH    | 34  | GLY  |
| 30  | BH    | 95  | GLY  |
| 32  | BK    | 15  | GLY  |
| 34  | BM    | 71  | LYS  |
| 34  | BM    | 131 | VAL  |
| 38  | BQ    | 7   | VAL  |
| 44  | BX    | 11  | VAL  |
| 3   | CD    | 27  | ILE  |
| 10  | CK    | 15  | VAL  |
| 12  | CM    | 42  | VAL  |
| 16  | CQ    | 32  | ILE  |
| 17  | CR    | 20  | ILE  |
| 25  | DC    | 48  | ILE  |
| 25  | DC    | 161 | VAL  |
| 30  | DH    | 4   | ILE  |
| 33  | DL    | 100 | ILE  |
| 41  | DT    | 58  | VAL  |
| 50  | D3    | 31  | ILE  |
| 50  | D3    | 62  | PRO  |
| 52  | DI    | 34  | ILE  |
| 3   | AD    | 63  | ILE  |
| 7   | AH    | 71  | VAL  |
| 8   | AI    | 71  | ILE  |
| 9   | AJ    | 41  | PRO  |
| 24  | BV    | 84  | PRO  |
| 25  | BC    | 234 | GLY  |
| 26  | BD    | 98  | VAL  |
| 27  | BE    | 113 | VAL  |
| 27  | BE    | 187 | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | BF    | 108 | PRO  |
| 30  | BH    | 110 | VAL  |
| 36  | BO    | 35  | ILE  |
| 37  | BP    | 69  | VAL  |
| 2   | CC    | 76  | ILE  |
| 2   | CC    | 107 | LYS  |
| 4   | CE    | 24  | VAL  |
| 20  | CB    | 123 | GLY  |
| 20  | CB    | 200 | PRO  |
| 25  | DC    | 54  | GLY  |
| 25  | DC    | 195 | GLY  |
| 26  | DD    | 19  | GLY  |
| 26  | DD    | 203 | VAL  |
| 33  | DL    | 23  | ILE  |
| 51  | D4    | 23  | ILE  |
| 3   | AD    | 37  | PRO  |
| 7   | AH    | 74  | ILE  |
| 8   | AI    | 110 | VAL  |
| 11  | AL    | 62  | VAL  |
| 12  | AM    | 15  | VAL  |
| 28  | BF    | 11  | VAL  |
| 29  | BG    | 8   | VAL  |
| 29  | BG    | 99  | GLY  |
| 33  | BL    | 16  | GLY  |
| 37  | BP    | 3   | ILE  |
| 8   | CI    | 68  | GLY  |
| 10  | CK    | 119 | GLY  |
| 16  | CQ    | 4   | ILE  |
| 25  | DC    | 16  | VAL  |
| 27  | DE    | 120 | VAL  |
| 28  | DF    | 108 | PRO  |
| 33  | DL    | 89  | VAL  |
| 36  | DO    | 31  | THR  |
| 36  | DO    | 58  | ILE  |
| 38  | DQ    | 6   | GLY  |
| 42  | DU    | 11  | ILE  |
| 47  | D0    | 53  | VAL  |
| 49  | D2    | 6   | GLN  |
| 8   | AI    | 39  | GLY  |
| 27  | BE    | 76  | PRO  |
| 34  | BM    | 89  | VAL  |
| 47  | B0    | 42  | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | DG    | 117 | PRO  |
| 30  | DH    | 32  | PRO  |
| 30  | DH    | 107 | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 2   | AC    | 170/190 (90%) | 152 (89%) | 18 (11%) | 6           | 27 |
| 2   | CC    | 170/190 (90%) | 151 (89%) | 19 (11%) | 6           | 26 |
| 3   | AD    | 172/173 (99%) | 145 (84%) | 27 (16%) | 2           | 15 |
| 3   | CD    | 172/173 (99%) | 146 (85%) | 26 (15%) | 3           | 17 |
| 4   | AE    | 113/126 (90%) | 99 (88%)  | 14 (12%) | 4           | 23 |
| 4   | CE    | 113/126 (90%) | 92 (81%)  | 21 (19%) | 1           | 9  |
| 5   | AF    | 87/116 (75%)  | 69 (79%)  | 18 (21%) | 1           | 6  |
| 5   | CF    | 87/116 (75%)  | 75 (86%)  | 12 (14%) | 3           | 19 |
| 6   | AG    | 123/147 (84%) | 108 (88%) | 15 (12%) | 5           | 23 |
| 6   | CG    | 125/147 (85%) | 112 (90%) | 13 (10%) | 7           | 28 |
| 7   | AH    | 104/105 (99%) | 94 (90%)  | 10 (10%) | 8           | 31 |
| 7   | CH    | 104/105 (99%) | 90 (86%)  | 14 (14%) | 4           | 20 |
| 8   | AI    | 105/107 (98%) | 87 (83%)  | 18 (17%) | 2           | 12 |
| 8   | CI    | 105/107 (98%) | 93 (89%)  | 12 (11%) | 5           | 25 |
| 9   | AJ    | 86/90 (96%)   | 73 (85%)  | 13 (15%) | 3           | 17 |
| 9   | CJ    | 86/90 (96%)   | 78 (91%)  | 8 (9%)   | 8           | 32 |
| 10  | AK    | 90/99 (91%)   | 75 (83%)  | 15 (17%) | 2           | 13 |
| 10  | CK    | 90/99 (91%)   | 79 (88%)  | 11 (12%) | 5           | 23 |
| 11  | AL    | 103/104 (99%) | 91 (88%)  | 12 (12%) | 5           | 25 |
| 11  | CL    | 103/104 (99%) | 83 (81%)  | 20 (19%) | 1           | 8  |
| 12  | AM    | 92/96 (96%)   | 78 (85%)  | 14 (15%) | 3           | 16 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 12  | CM    | 91/96 (95%)    | 80 (88%)  | 11 (12%) | 5           | 23 |
| 13  | AN    | 79/84 (94%)    | 68 (86%)  | 11 (14%) | 3           | 19 |
| 13  | CN    | 79/84 (94%)    | 68 (86%)  | 11 (14%) | 3           | 19 |
| 14  | AO    | 76/77 (99%)    | 70 (92%)  | 6 (8%)   | 11          | 37 |
| 14  | CO    | 76/77 (99%)    | 66 (87%)  | 10 (13%) | 4           | 21 |
| 15  | AP    | 65/65 (100%)   | 54 (83%)  | 11 (17%) | 2           | 13 |
| 15  | CP    | 65/65 (100%)   | 57 (88%)  | 8 (12%)  | 4           | 23 |
| 16  | AQ    | 74/78 (95%)    | 63 (85%)  | 11 (15%) | 3           | 17 |
| 16  | CQ    | 75/78 (96%)    | 67 (89%)  | 8 (11%)  | 6           | 27 |
| 17  | AR    | 48/65 (74%)    | 43 (90%)  | 5 (10%)  | 7           | 28 |
| 17  | CR    | 48/65 (74%)    | 43 (90%)  | 5 (10%)  | 7           | 28 |
| 18  | AS    | 70/79 (89%)    | 64 (91%)  | 6 (9%)   | 10          | 34 |
| 18  | CS    | 71/79 (90%)    | 59 (83%)  | 12 (17%) | 2           | 13 |
| 19  | AT    | 65/66 (98%)    | 56 (86%)  | 9 (14%)  | 3           | 19 |
| 19  | CT    | 65/66 (98%)    | 54 (83%)  | 11 (17%) | 2           | 13 |
| 20  | AB    | 180/199 (90%)  | 149 (83%) | 31 (17%) | 2           | 12 |
| 20  | CB    | 180/199 (90%)  | 155 (86%) | 25 (14%) | 3           | 19 |
| 21  | AU    | 44/61 (72%)    | 41 (93%)  | 3 (7%)   | 14          | 41 |
| 21  | CU    | 44/61 (72%)    | 35 (80%)  | 9 (20%)  | 1           | 7  |
| 24  | BV    | 78/78 (100%)   | 66 (85%)  | 12 (15%) | 2           | 16 |
| 24  | DV    | 78/78 (100%)   | 71 (91%)  | 7 (9%)   | 9           | 33 |
| 25  | BC    | 213/218 (98%)  | 161 (76%) | 52 (24%) | 1           | 4  |
| 25  | DC    | 213/218 (98%)  | 163 (76%) | 50 (24%) | 1           | 4  |
| 26  | BD    | 164/164 (100%) | 122 (74%) | 42 (26%) | 0           | 3  |
| 26  | DD    | 164/164 (100%) | 126 (77%) | 38 (23%) | 1           | 5  |
| 27  | BE    | 165/165 (100%) | 127 (77%) | 38 (23%) | 1           | 5  |
| 27  | DE    | 165/165 (100%) | 138 (84%) | 27 (16%) | 2           | 14 |
| 28  | BF    | 149/150 (99%)  | 130 (87%) | 19 (13%) | 4           | 22 |
| 28  | DF    | 149/150 (99%)  | 126 (85%) | 23 (15%) | 2           | 16 |
| 29  | BG    | 137/138 (99%)  | 114 (83%) | 23 (17%) | 2           | 13 |
| 29  | DG    | 137/138 (99%)  | 115 (84%) | 22 (16%) | 2           | 14 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 30  | BH    | 114/114 (100%) | 97 (85%)  | 17 (15%) | 3           | 17 |
| 30  | DH    | 114/114 (100%) | 95 (83%)  | 19 (17%) | 2           | 13 |
| 31  | BJ    | 114/116 (98%)  | 95 (83%)  | 19 (17%) | 2           | 13 |
| 31  | DJ    | 114/116 (98%)  | 91 (80%)  | 23 (20%) | 1           | 7  |
| 32  | BK    | 102/104 (98%)  | 82 (80%)  | 20 (20%) | 1           | 8  |
| 32  | DK    | 102/104 (98%)  | 90 (88%)  | 12 (12%) | 5           | 24 |
| 33  | BL    | 103/103 (100%) | 75 (73%)  | 28 (27%) | 0           | 3  |
| 33  | DL    | 103/103 (100%) | 69 (67%)  | 34 (33%) | 0           | 2  |
| 34  | BM    | 109/109 (100%) | 83 (76%)  | 26 (24%) | 1           | 4  |
| 34  | DM    | 109/109 (100%) | 78 (72%)  | 31 (28%) | 0           | 3  |
| 35  | BN    | 103/103 (100%) | 86 (84%)  | 17 (16%) | 2           | 14 |
| 35  | DN    | 103/103 (100%) | 84 (82%)  | 19 (18%) | 1           | 9  |
| 36  | BO    | 87/87 (100%)   | 70 (80%)  | 17 (20%) | 1           | 8  |
| 36  | DO    | 87/87 (100%)   | 75 (86%)  | 12 (14%) | 3           | 19 |
| 37  | BP    | 99/100 (99%)   | 75 (76%)  | 24 (24%) | 1           | 4  |
| 37  | DP    | 99/100 (99%)   | 69 (70%)  | 30 (30%) | 0           | 2  |
| 38  | BQ    | 89/90 (99%)    | 71 (80%)  | 18 (20%) | 1           | 7  |
| 38  | DQ    | 89/90 (99%)    | 72 (81%)  | 17 (19%) | 1           | 8  |
| 39  | BR    | 84/84 (100%)   | 73 (87%)  | 11 (13%) | 4           | 21 |
| 39  | DR    | 84/84 (100%)   | 67 (80%)  | 17 (20%) | 1           | 7  |
| 40  | BS    | 93/93 (100%)   | 83 (89%)  | 10 (11%) | 6           | 27 |
| 40  | DS    | 93/93 (100%)   | 80 (86%)  | 13 (14%) | 3           | 19 |
| 41  | BT    | 83/84 (99%)    | 66 (80%)  | 17 (20%) | 1           | 7  |
| 41  | DT    | 83/84 (99%)    | 69 (83%)  | 14 (17%) | 2           | 13 |
| 42  | BU    | 83/85 (98%)    | 65 (78%)  | 18 (22%) | 1           | 6  |
| 42  | DU    | 83/85 (98%)    | 64 (77%)  | 19 (23%) | 1           | 5  |
| 43  | BW    | 62/63 (98%)    | 50 (81%)  | 12 (19%) | 1           | 8  |
| 43  | DW    | 62/63 (98%)    | 49 (79%)  | 13 (21%) | 1           | 6  |
| 44  | BX    | 55/55 (100%)   | 40 (73%)  | 15 (27%) | 0           | 3  |
| 44  | DX    | 55/55 (100%)   | 45 (82%)  | 10 (18%) | 2           | 10 |
| 45  | BY    | 48/49 (98%)    | 37 (77%)  | 11 (23%) | 1           | 5  |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Analysed        | Rotameric  | Outliers   | Percentiles |    |
|-----|-------|-----------------|------------|------------|-------------|----|
| 45  | DY    | 48/49 (98%)     | 38 (79%)   | 10 (21%)   | 1           | 6  |
| 46  | BZ    | 62/62 (100%)    | 45 (73%)   | 17 (27%)   | 0           | 3  |
| 46  | DZ    | 62/62 (100%)    | 54 (87%)   | 8 (13%)    | 4           | 21 |
| 47  | B0    | 47/48 (98%)     | 38 (81%)   | 9 (19%)    | 1           | 8  |
| 47  | D0    | 47/48 (98%)     | 38 (81%)   | 9 (19%)    | 1           | 8  |
| 48  | B1    | 48/49 (98%)     | 33 (69%)   | 15 (31%)   | 0           | 2  |
| 48  | D1    | 48/49 (98%)     | 38 (79%)   | 10 (21%)   | 1           | 6  |
| 49  | B2    | 38/38 (100%)    | 33 (87%)   | 5 (13%)    | 4           | 21 |
| 49  | D2    | 38/38 (100%)    | 29 (76%)   | 9 (24%)    | 1           | 4  |
| 50  | B3    | 51/52 (98%)     | 39 (76%)   | 12 (24%)   | 1           | 4  |
| 50  | D3    | 51/52 (98%)     | 41 (80%)   | 10 (20%)   | 1           | 8  |
| 51  | B4    | 34/34 (100%)    | 25 (74%)   | 9 (26%)    | 0           | 3  |
| 51  | D4    | 34/34 (100%)    | 21 (62%)   | 13 (38%)   | 0           | 1  |
| 52  | BI    | 109/110 (99%)   | 108 (99%)  | 1 (1%)     | 70          | 76 |
| 52  | DI    | 109/110 (99%)   | 105 (96%)  | 4 (4%)     | 30          | 57 |
| All | All   | 9341/9744 (96%) | 7751 (83%) | 1590 (17%) | 2           | 12 |

All (1590) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AC    | 14  | VAL  |
| 2   | AC    | 31  | ASN  |
| 2   | AC    | 40  | GLN  |
| 2   | AC    | 42  | LEU  |
| 2   | AC    | 100 | ILE  |
| 2   | AC    | 102 | ILE  |
| 2   | AC    | 113 | LYS  |
| 2   | AC    | 141 | MET  |
| 2   | AC    | 143 | LEU  |
| 2   | AC    | 146 | LYS  |
| 2   | AC    | 156 | LEU  |
| 2   | AC    | 165 | GLU  |
| 2   | AC    | 166 | TRP  |
| 2   | AC    | 180 | ASP  |
| 2   | AC    | 189 | HIS  |
| 2   | AC    | 190 | THR  |
| 2   | AC    | 192 | TYR  |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AC    | 205 | GLU  |
| 3   | AD    | 7   | LYS  |
| 3   | AD    | 8   | LEU  |
| 3   | AD    | 10  | LEU  |
| 3   | AD    | 21  | LYS  |
| 3   | AD    | 25  | ARG  |
| 3   | AD    | 35  | GLN  |
| 3   | AD    | 39  | GLN  |
| 3   | AD    | 54  | LEU  |
| 3   | AD    | 56  | GLU  |
| 3   | AD    | 58  | GLN  |
| 3   | AD    | 69  | ARG  |
| 3   | AD    | 85  | THR  |
| 3   | AD    | 87  | GLU  |
| 3   | AD    | 94  | GLU  |
| 3   | AD    | 147 | LYS  |
| 3   | AD    | 150 | LYS  |
| 3   | AD    | 153 | ARG  |
| 3   | AD    | 154 | VAL  |
| 3   | AD    | 155 | LYS  |
| 3   | AD    | 158 | LEU  |
| 3   | AD    | 159 | GLU  |
| 3   | AD    | 160 | LEU  |
| 3   | AD    | 162 | GLU  |
| 3   | AD    | 176 | LYS  |
| 3   | AD    | 177 | MET  |
| 3   | AD    | 183 | ARG  |
| 3   | AD    | 194 | ILE  |
| 4   | AE    | 11  | GLN  |
| 4   | AE    | 23  | THR  |
| 4   | AE    | 25  | LYS  |
| 4   | AE    | 68  | ARG  |
| 4   | AE    | 81  | GLN  |
| 4   | AE    | 102 | THR  |
| 4   | AE    | 110 | MET  |
| 4   | AE    | 122 | VAL  |
| 4   | AE    | 123 | LEU  |
| 4   | AE    | 125 | LYS  |
| 4   | AE    | 139 | THR  |
| 4   | AE    | 143 | LEU  |
| 4   | AE    | 151 | MET  |
| 4   | AE    | 158 | LYS  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | AF    | 6   | ILE  |
| 5   | AF    | 37  | HIS  |
| 5   | AF    | 38  | ARG  |
| 5   | AF    | 39  | LEU  |
| 5   | AF    | 46  | GLN  |
| 5   | AF    | 53  | LYS  |
| 5   | AF    | 54  | LEU  |
| 5   | AF    | 55  | HIS  |
| 5   | AF    | 61  | LEU  |
| 5   | AF    | 65  | GLU  |
| 5   | AF    | 68  | GLN  |
| 5   | AF    | 69  | GLU  |
| 5   | AF    | 71  | ILE  |
| 5   | AF    | 75  | GLU  |
| 5   | AF    | 76  | THR  |
| 5   | AF    | 78  | PHE  |
| 5   | AF    | 88  | MET  |
| 5   | AF    | 92  | THR  |
| 6   | AG    | 3   | ARG  |
| 6   | AG    | 10  | LYS  |
| 6   | AG    | 11  | ILE  |
| 6   | AG    | 14  | ASP  |
| 6   | AG    | 16  | LYS  |
| 6   | AG    | 21  | LEU  |
| 6   | AG    | 22  | LEU  |
| 6   | AG    | 29  | LEU  |
| 6   | AG    | 42  | VAL  |
| 6   | AG    | 68  | VAL  |
| 6   | AG    | 72  | VAL  |
| 6   | AG    | 74  | VAL  |
| 6   | AG    | 84  | TYR  |
| 6   | AG    | 89  | GLU  |
| 6   | AG    | 119 | LEU  |
| 7   | AH    | 30  | LYS  |
| 7   | AH    | 39  | LEU  |
| 7   | AH    | 55  | LYS  |
| 7   | AH    | 58  | LEU  |
| 7   | AH    | 60  | LEU  |
| 7   | AH    | 82  | LEU  |
| 7   | AH    | 93  | LYS  |
| 7   | AH    | 111 | THR  |
| 7   | AH    | 113 | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | AH    | 120 | LEU  |
| 8   | AI    | 11  | ARG  |
| 8   | AI    | 26  | LYS  |
| 8   | AI    | 30  | ASN  |
| 8   | AI    | 36  | GLN  |
| 8   | AI    | 38  | PHE  |
| 8   | AI    | 41  | GLU  |
| 8   | AI    | 44  | ARG  |
| 8   | AI    | 56  | MET  |
| 8   | AI    | 58  | GLU  |
| 8   | AI    | 59  | LYS  |
| 8   | AI    | 62  | LEU  |
| 8   | AI    | 84  | ARG  |
| 8   | AI    | 86  | LEU  |
| 8   | AI    | 87  | MET  |
| 8   | AI    | 106 | ASP  |
| 8   | AI    | 119 | LYS  |
| 8   | AI    | 121 | ARG  |
| 8   | AI    | 126 | PHE  |
| 9   | AJ    | 11  | LYS  |
| 9   | AJ    | 18  | ILE  |
| 9   | AJ    | 40  | ILE  |
| 9   | AJ    | 48  | ARG  |
| 9   | AJ    | 49  | PHE  |
| 9   | AJ    | 57  | VAL  |
| 9   | AJ    | 71  | LEU  |
| 9   | AJ    | 75  | ASP  |
| 9   | AJ    | 81  | GLU  |
| 9   | AJ    | 88  | MET  |
| 9   | AJ    | 89  | ARG  |
| 9   | AJ    | 92  | LEU  |
| 9   | AJ    | 102 | LEU  |
| 10  | AK    | 36  | ARG  |
| 10  | AK    | 37  | GLN  |
| 10  | AK    | 52  | ARG  |
| 10  | AK    | 56  | LYS  |
| 10  | AK    | 58  | THR  |
| 10  | AK    | 60  | PHE  |
| 10  | AK    | 73  | VAL  |
| 10  | AK    | 74  | LYS  |
| 10  | AK    | 83  | VAL  |
| 10  | AK    | 84  | MET  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | AK    | 92  | ARG  |
| 10  | AK    | 99  | LEU  |
| 10  | AK    | 107 | THR  |
| 10  | AK    | 108 | ASN  |
| 10  | AK    | 115 | ILE  |
| 11  | AL    | 20  | VAL  |
| 11  | AL    | 24  | GLU  |
| 11  | AL    | 28  | GLN  |
| 11  | AL    | 30  | ARG  |
| 11  | AL    | 35  | ARG  |
| 11  | AL    | 38  | THR  |
| 11  | AL    | 48  | LEU  |
| 11  | AL    | 50  | LYS  |
| 11  | AL    | 58  | ASN  |
| 11  | AL    | 71  | HIS  |
| 11  | AL    | 74  | GLN  |
| 11  | AL    | 87  | LYS  |
| 12  | AM    | 18  | LEU  |
| 12  | AM    | 41  | ASP  |
| 12  | AM    | 44  | ILE  |
| 12  | AM    | 57  | ASP  |
| 12  | AM    | 62  | PHE  |
| 12  | AM    | 64  | VAL  |
| 12  | AM    | 67  | ASP  |
| 12  | AM    | 68  | LEU  |
| 12  | AM    | 90  | HIS  |
| 12  | AM    | 99  | GLN  |
| 12  | AM    | 101 | THR  |
| 12  | AM    | 102 | LYS  |
| 12  | AM    | 106 | ARG  |
| 12  | AM    | 109 | LYS  |
| 13  | AN    | 11  | LYS  |
| 13  | AN    | 15  | LEU  |
| 13  | AN    | 27  | LYS  |
| 13  | AN    | 41  | TRP  |
| 13  | AN    | 47  | LEU  |
| 13  | AN    | 50  | LEU  |
| 13  | AN    | 59  | GLN  |
| 13  | AN    | 65  | GLN  |
| 13  | AN    | 73  | LEU  |
| 13  | AN    | 74  | ARG  |
| 13  | AN    | 81  | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | AO    | 7   | THR  |
| 14  | AO    | 17  | ASP  |
| 14  | AO    | 25  | GLU  |
| 14  | AO    | 53  | ARG  |
| 14  | AO    | 58  | MET  |
| 14  | AO    | 70  | LYS  |
| 15  | AP    | 4   | ILE  |
| 15  | AP    | 5   | ARG  |
| 15  | AP    | 19  | VAL  |
| 15  | AP    | 21  | VAL  |
| 15  | AP    | 26  | ASN  |
| 15  | AP    | 29  | ASN  |
| 15  | AP    | 31  | ARG  |
| 15  | AP    | 34  | GLU  |
| 15  | AP    | 46  | LYS  |
| 15  | AP    | 55  | ASP  |
| 15  | AP    | 63  | GLN  |
| 16  | AQ    | 4   | ILE  |
| 16  | AQ    | 10  | ARG  |
| 16  | AQ    | 20  | ILE  |
| 16  | AQ    | 25  | GLU  |
| 16  | AQ    | 39  | ARG  |
| 16  | AQ    | 47  | ASP  |
| 16  | AQ    | 60  | ILE  |
| 16  | AQ    | 74  | LEU  |
| 16  | AQ    | 76  | ARG  |
| 16  | AQ    | 78  | VAL  |
| 16  | AQ    | 80  | LYS  |
| 17  | AR    | 20  | ILE  |
| 17  | AR    | 23  | LYS  |
| 17  | AR    | 30  | ASN  |
| 17  | AR    | 43  | ILE  |
| 17  | AR    | 52  | ARG  |
| 18  | AS    | 5   | LYS  |
| 18  | AS    | 20  | LYS  |
| 18  | AS    | 35  | ARG  |
| 18  | AS    | 40  | PHE  |
| 18  | AS    | 47  | THR  |
| 18  | AS    | 72  | GLU  |
| 19  | AT    | 14  | GLU  |
| 19  | AT    | 29  | THR  |
| 19  | AT    | 34  | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | AT    | 38  | ILE  |
| 19  | AT    | 43  | LYS  |
| 19  | AT    | 59  | ARG  |
| 19  | AT    | 67  | HIS  |
| 19  | AT    | 70  | LYS  |
| 19  | AT    | 85  | LEU  |
| 20  | AB    | 9   | LEU  |
| 20  | AB    | 18  | GLN  |
| 20  | AB    | 22  | TRP  |
| 20  | AB    | 36  | LYS  |
| 20  | AB    | 38  | HIS  |
| 20  | AB    | 40  | ILE  |
| 20  | AB    | 46  | VAL  |
| 20  | AB    | 48  | MET  |
| 20  | AB    | 56  | LEU  |
| 20  | AB    | 57  | ASN  |
| 20  | AB    | 58  | LYS  |
| 20  | AB    | 67  | LEU  |
| 20  | AB    | 81  | ASP  |
| 20  | AB    | 88  | GLN  |
| 20  | AB    | 90  | PHE  |
| 20  | AB    | 94  | ARG  |
| 20  | AB    | 95  | TRP  |
| 20  | AB    | 116 | LEU  |
| 20  | AB    | 121 | GLN  |
| 20  | AB    | 122 | ASP  |
| 20  | AB    | 125 | PHE  |
| 20  | AB    | 127 | LYS  |
| 20  | AB    | 128 | LEU  |
| 20  | AB    | 145 | ASN  |
| 20  | AB    | 176 | ASN  |
| 20  | AB    | 185 | ILE  |
| 20  | AB    | 188 | THR  |
| 20  | AB    | 196 | ASP  |
| 20  | AB    | 202 | ASN  |
| 20  | AB    | 206 | ILE  |
| 20  | AB    | 222 | GLU  |
| 21  | AU    | 11  | PHE  |
| 21  | AU    | 12  | ASP  |
| 21  | AU    | 41  | THR  |
| 24  | BV    | 3   | THR  |
| 24  | BV    | 9   | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | BV    | 35  | GLU  |
| 24  | BV    | 40  | ILE  |
| 24  | BV    | 42  | LEU  |
| 24  | BV    | 46  | LYS  |
| 24  | BV    | 51  | GLN  |
| 24  | BV    | 70  | ILE  |
| 24  | BV    | 73  | LYS  |
| 24  | BV    | 79  | ARG  |
| 24  | BV    | 82  | TYR  |
| 24  | BV    | 87  | GLN  |
| 25  | BC    | 5   | CYS  |
| 25  | BC    | 14  | HIS  |
| 25  | BC    | 17  | LYS  |
| 25  | BC    | 18  | VAL  |
| 25  | BC    | 27  | LYS  |
| 25  | BC    | 28  | PRO  |
| 25  | BC    | 32  | LEU  |
| 25  | BC    | 33  | LEU  |
| 25  | BC    | 35  | LYS  |
| 25  | BC    | 36  | ASN  |
| 25  | BC    | 38  | LYS  |
| 25  | BC    | 43  | ASN  |
| 25  | BC    | 45  | ASN  |
| 25  | BC    | 51  | ARG  |
| 25  | BC    | 57  | HIS  |
| 25  | BC    | 58  | LYS  |
| 25  | BC    | 62  | ARG  |
| 25  | BC    | 64  | VAL  |
| 25  | BC    | 78  | GLU  |
| 25  | BC    | 86  | ARG  |
| 25  | BC    | 94  | LEU  |
| 25  | BC    | 102 | TYR  |
| 25  | BC    | 110 | LYS  |
| 25  | BC    | 125 | PRO  |
| 25  | BC    | 127 | ASN  |
| 25  | BC    | 129 | LEU  |
| 25  | BC    | 131 | MET  |
| 25  | BC    | 144 | GLU  |
| 25  | BC    | 152 | GLN  |
| 25  | BC    | 155 | ARG  |
| 25  | BC    | 162 | GLN  |
| 25  | BC    | 171 | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | BC    | 180 | MET  |
| 25  | BC    | 186 | ASP  |
| 25  | BC    | 199 | HIS  |
| 25  | BC    | 201 | LEU  |
| 25  | BC    | 203 | VAL  |
| 25  | BC    | 206 | LYS  |
| 25  | BC    | 220 | ARG  |
| 25  | BC    | 222 | THR  |
| 25  | BC    | 224 | MET  |
| 25  | BC    | 225 | ASN  |
| 25  | BC    | 227 | VAL  |
| 25  | BC    | 231 | HIS  |
| 25  | BC    | 235 | GLU  |
| 25  | BC    | 237 | ARG  |
| 25  | BC    | 244 | VAL  |
| 25  | BC    | 246 | PRO  |
| 25  | BC    | 256 | THR  |
| 25  | BC    | 257 | ARG  |
| 25  | BC    | 263 | ASP  |
| 25  | BC    | 268 | ARG  |
| 26  | BD    | 8   | LYS  |
| 26  | BD    | 17  | GLU  |
| 26  | BD    | 18  | ASP  |
| 26  | BD    | 25  | THR  |
| 26  | BD    | 28  | GLU  |
| 26  | BD    | 29  | VAL  |
| 26  | BD    | 30  | GLU  |
| 26  | BD    | 32  | ASN  |
| 26  | BD    | 35  | THR  |
| 26  | BD    | 36  | GLN  |
| 26  | BD    | 38  | LYS  |
| 26  | BD    | 39  | ASP  |
| 26  | BD    | 48  | ILE  |
| 26  | BD    | 52  | THR  |
| 26  | BD    | 55  | LYS  |
| 26  | BD    | 56  | LYS  |
| 26  | BD    | 59  | ARG  |
| 26  | BD    | 62  | LYS  |
| 26  | BD    | 67  | HIS  |
| 26  | BD    | 70  | LYS  |
| 26  | BD    | 96  | ILE  |
| 26  | BD    | 99  | GLU  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | BD    | 103 | ASP  |
| 26  | BD    | 105 | LYS  |
| 26  | BD    | 107 | VAL  |
| 26  | BD    | 123 | LYS  |
| 26  | BD    | 127 | PHE  |
| 26  | BD    | 128 | ARG  |
| 26  | BD    | 131 | ASP  |
| 26  | BD    | 133 | THR  |
| 26  | BD    | 138 | LEU  |
| 26  | BD    | 140 | HIS  |
| 26  | BD    | 141 | ARG  |
| 26  | BD    | 146 | ILE  |
| 26  | BD    | 148 | GLN  |
| 26  | BD    | 155 | VAL  |
| 26  | BD    | 157 | LYS  |
| 26  | BD    | 159 | LYS  |
| 26  | BD    | 160 | LYS  |
| 26  | BD    | 167 | ASN  |
| 26  | BD    | 177 | VAL  |
| 26  | BD    | 197 | THR  |
| 27  | BE    | 4   | VAL  |
| 27  | BE    | 5   | LEU  |
| 27  | BE    | 10  | SER  |
| 27  | BE    | 18  | THR  |
| 27  | BE    | 22  | ASP  |
| 27  | BE    | 24  | ASN  |
| 27  | BE    | 41  | GLN  |
| 27  | BE    | 43  | THR  |
| 27  | BE    | 44  | ARG  |
| 27  | BE    | 46  | GLN  |
| 27  | BE    | 47  | LYS  |
| 27  | BE    | 49  | ARG  |
| 27  | BE    | 57  | LYS  |
| 27  | BE    | 58  | LYS  |
| 27  | BE    | 59  | PRO  |
| 27  | BE    | 67  | ARG  |
| 27  | BE    | 78  | TRP  |
| 27  | BE    | 85  | PHE  |
| 27  | BE    | 88  | ARG  |
| 27  | BE    | 98  | LYS  |
| 27  | BE    | 106 | LYS  |
| 27  | BE    | 113 | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | BE    | 118 | LEU  |
| 27  | BE    | 132 | LYS  |
| 27  | BE    | 134 | LEU  |
| 27  | BE    | 139 | LYS  |
| 27  | BE    | 143 | LEU  |
| 27  | BE    | 148 | ILE  |
| 27  | BE    | 149 | ILE  |
| 27  | BE    | 164 | LEU  |
| 27  | BE    | 169 | VAL  |
| 27  | BE    | 184 | ASP  |
| 27  | BE    | 188 | MET  |
| 27  | BE    | 189 | THR  |
| 27  | BE    | 193 | VAL  |
| 27  | BE    | 196 | VAL  |
| 27  | BE    | 199 | MET  |
| 27  | BE    | 200 | LEU  |
| 28  | BF    | 5   | ASP  |
| 28  | BF    | 14  | LYS  |
| 28  | BF    | 16  | MET  |
| 28  | BF    | 21  | TYR  |
| 28  | BF    | 55  | ASP  |
| 28  | BF    | 56  | LEU  |
| 28  | BF    | 59  | ILE  |
| 28  | BF    | 93  | GLU  |
| 28  | BF    | 126 | ASN  |
| 28  | BF    | 132 | ARG  |
| 28  | BF    | 139 | GLU  |
| 28  | BF    | 142 | TYR  |
| 28  | BF    | 143 | ASP  |
| 28  | BF    | 146 | ASP  |
| 28  | BF    | 147 | ARG  |
| 28  | BF    | 157 | THR  |
| 28  | BF    | 166 | ARG  |
| 28  | BF    | 168 | LEU  |
| 28  | BF    | 177 | ARG  |
| 29  | BG    | 2   | ARG  |
| 29  | BG    | 3   | VAL  |
| 29  | BG    | 18  | ILE  |
| 29  | BG    | 23  | ILE  |
| 29  | BG    | 28  | LYS  |
| 29  | BG    | 34  | ARG  |
| 29  | BG    | 46  | ASP  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | BG    | 49  | LEU  |
| 29  | BG    | 50  | THR  |
| 29  | BG    | 57  | TYR  |
| 29  | BG    | 59  | ASP  |
| 29  | BG    | 70  | LEU  |
| 29  | BG    | 84  | LYS  |
| 29  | BG    | 86  | LEU  |
| 29  | BG    | 94  | ARG  |
| 29  | BG    | 121 | THR  |
| 29  | BG    | 128 | THR  |
| 29  | BG    | 146 | ASP  |
| 29  | BG    | 150 | TYR  |
| 29  | BG    | 152 | ARG  |
| 29  | BG    | 154 | GLU  |
| 29  | BG    | 172 | GLU  |
| 29  | BG    | 176 | LYS  |
| 30  | BH    | 5   | LEU  |
| 30  | BH    | 7   | ASP  |
| 30  | BH    | 8   | LYS  |
| 30  | BH    | 22  | LYS  |
| 30  | BH    | 28  | ASN  |
| 30  | BH    | 30  | LEU  |
| 30  | BH    | 35  | LYS  |
| 30  | BH    | 42  | LYS  |
| 30  | BH    | 55  | GLU  |
| 30  | BH    | 57  | LYS  |
| 30  | BH    | 66  | ASN  |
| 30  | BH    | 70  | GLU  |
| 30  | BH    | 73  | ASN  |
| 30  | BH    | 75  | LEU  |
| 30  | BH    | 89  | LYS  |
| 30  | BH    | 112 | LYS  |
| 30  | BH    | 132 | PHE  |
| 31  | BJ    | 12  | LYS  |
| 31  | BJ    | 15  | TRP  |
| 31  | BJ    | 23  | LYS  |
| 31  | BJ    | 24  | THR  |
| 31  | BJ    | 25  | LEU  |
| 31  | BJ    | 28  | LEU  |
| 31  | BJ    | 34  | ARG  |
| 31  | BJ    | 35  | ARG  |
| 31  | BJ    | 39  | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | BJ    | 58  | ASN  |
| 31  | BJ    | 61  | LYS  |
| 31  | BJ    | 64  | VAL  |
| 31  | BJ    | 75  | TYR  |
| 31  | BJ    | 90  | GLU  |
| 31  | BJ    | 96  | ARG  |
| 31  | BJ    | 98  | GLU  |
| 31  | BJ    | 114 | LEU  |
| 31  | BJ    | 122 | LEU  |
| 31  | BJ    | 136 | GLN  |
| 32  | BK    | 9   | ASN  |
| 32  | BK    | 17  | ARG  |
| 32  | BK    | 19  | VAL  |
| 32  | BK    | 30  | ARG  |
| 32  | BK    | 31  | ARG  |
| 32  | BK    | 32  | TYR  |
| 32  | BK    | 41  | ILE  |
| 32  | BK    | 45  | GLU  |
| 32  | BK    | 47  | ILE  |
| 32  | BK    | 54  | LYS  |
| 32  | BK    | 58  | LEU  |
| 32  | BK    | 62  | VAL  |
| 32  | BK    | 71  | ARG  |
| 32  | BK    | 79  | PHE  |
| 32  | BK    | 87  | LEU  |
| 32  | BK    | 108 | ARG  |
| 32  | BK    | 109 | SER  |
| 32  | BK    | 113 | MET  |
| 32  | BK    | 116 | ILE  |
| 32  | BK    | 118 | LEU  |
| 33  | BL    | 2   | ARG  |
| 33  | BL    | 14  | LYS  |
| 33  | BL    | 18  | ARG  |
| 33  | BL    | 27  | LEU  |
| 33  | BL    | 29  | LYS  |
| 33  | BL    | 33  | ARG  |
| 33  | BL    | 41  | ARG  |
| 33  | BL    | 47  | ARG  |
| 33  | BL    | 51  | GLU  |
| 33  | BL    | 55  | MET  |
| 33  | BL    | 61  | LEU  |
| 33  | BL    | 62  | PRO  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | BL    | 70  | LYS  |
| 33  | BL    | 78  | ARG  |
| 33  | BL    | 82  | LEU  |
| 33  | BL    | 84  | LYS  |
| 33  | BL    | 85  | VAL  |
| 33  | BL    | 96  | LYS  |
| 33  | BL    | 103 | ILE  |
| 33  | BL    | 105 | ILE  |
| 33  | BL    | 106 | GLU  |
| 33  | BL    | 110 | VAL  |
| 33  | BL    | 111 | ILE  |
| 33  | BL    | 112 | LEU  |
| 33  | BL    | 116 | VAL  |
| 33  | BL    | 118 | THR  |
| 33  | BL    | 127 | VAL  |
| 33  | BL    | 132 | ARG  |
| 34  | BM    | 3   | GLN  |
| 34  | BM    | 9   | PHE  |
| 34  | BM    | 11  | LYS  |
| 34  | BM    | 12  | MET  |
| 34  | BM    | 14  | LYS  |
| 34  | BM    | 17  | ASN  |
| 34  | BM    | 18  | ARG  |
| 34  | BM    | 22  | GLN  |
| 34  | BM    | 36  | VAL  |
| 34  | BM    | 38  | ARG  |
| 34  | BM    | 54  | THR  |
| 34  | BM    | 55  | ARG  |
| 34  | BM    | 63  | ILE  |
| 34  | BM    | 71  | LYS  |
| 34  | BM    | 84  | LYS  |
| 34  | BM    | 86  | LYS  |
| 34  | BM    | 93  | VAL  |
| 34  | BM    | 96  | ILE  |
| 34  | BM    | 100 | LYS  |
| 34  | BM    | 109 | PRO  |
| 34  | BM    | 110 | GLU  |
| 34  | BM    | 117 | PHE  |
| 34  | BM    | 118 | LYS  |
| 34  | BM    | 130 | PHE  |
| 34  | BM    | 133 | LYS  |
| 34  | BM    | 135 | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | BN    | 1   | MET  |
| 35  | BN    | 9   | GLN  |
| 35  | BN    | 10  | LEU  |
| 35  | BN    | 13  | ASN  |
| 35  | BN    | 21  | PHE  |
| 35  | BN    | 33  | ILE  |
| 35  | BN    | 34  | ILE  |
| 35  | BN    | 35  | LYS  |
| 35  | BN    | 38  | LEU  |
| 35  | BN    | 47  | VAL  |
| 35  | BN    | 57  | THR  |
| 35  | BN    | 75  | ILE  |
| 35  | BN    | 76  | VAL  |
| 35  | BN    | 99  | LYS  |
| 35  | BN    | 102 | PHE  |
| 35  | BN    | 112 | TYR  |
| 35  | BN    | 120 | GLU  |
| 36  | BO    | 1   | MET  |
| 36  | BO    | 3   | LYS  |
| 36  | BO    | 8   | ILE  |
| 36  | BO    | 13  | ARG  |
| 36  | BO    | 25  | ARG  |
| 36  | BO    | 31  | THR  |
| 36  | BO    | 32  | PRO  |
| 36  | BO    | 35  | ILE  |
| 36  | BO    | 40  | ILE  |
| 36  | BO    | 56  | LYS  |
| 36  | BO    | 58  | ILE  |
| 36  | BO    | 62  | LEU  |
| 36  | BO    | 64  | TYR  |
| 36  | BO    | 69  | ASP  |
| 36  | BO    | 84  | GLU  |
| 36  | BO    | 98  | GLN  |
| 36  | BO    | 116 | GLN  |
| 37  | BP    | 2   | ASN  |
| 37  | BP    | 8   | GLU  |
| 37  | BP    | 15  | ASP  |
| 37  | BP    | 24  | THR  |
| 37  | BP    | 30  | TRP  |
| 37  | BP    | 38  | ARG  |
| 37  | BP    | 46  | VAL  |
| 37  | BP    | 47  | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | BP    | 49  | ILE  |
| 37  | BP    | 50  | ARG  |
| 37  | BP    | 52  | ARG  |
| 37  | BP    | 54  | LEU  |
| 37  | BP    | 55  | HIS  |
| 37  | BP    | 60  | VAL  |
| 37  | BP    | 62  | LYS  |
| 37  | BP    | 74  | GLN  |
| 37  | BP    | 87  | ARG  |
| 37  | BP    | 88  | ARG  |
| 37  | BP    | 96  | LEU  |
| 37  | BP    | 101 | GLU  |
| 37  | BP    | 108 | ARG  |
| 37  | BP    | 112 | ARG  |
| 37  | BP    | 113 | LEU  |
| 37  | BP    | 114 | ASN  |
| 38  | BQ    | 3   | VAL  |
| 38  | BQ    | 5   | ARG  |
| 38  | BQ    | 36  | GLN  |
| 38  | BQ    | 38  | VAL  |
| 38  | BQ    | 39  | ILE  |
| 38  | BQ    | 51  | GLN  |
| 38  | BQ    | 63  | ARG  |
| 38  | BQ    | 65  | ASN  |
| 38  | BQ    | 70  | GLN  |
| 38  | BQ    | 71  | ASN  |
| 38  | BQ    | 80  | ASN  |
| 38  | BQ    | 84  | LYS  |
| 38  | BQ    | 92  | LYS  |
| 38  | BQ    | 94  | LEU  |
| 38  | BQ    | 101 | ASP  |
| 38  | BQ    | 102 | LYS  |
| 38  | BQ    | 108 | LEU  |
| 38  | BQ    | 113 | LYS  |
| 39  | BR    | 12  | HIS  |
| 39  | BR    | 13  | ARG  |
| 39  | BR    | 18  | GLN  |
| 39  | BR    | 20  | VAL  |
| 39  | BR    | 23  | GLU  |
| 39  | BR    | 62  | GLU  |
| 39  | BR    | 70  | GLU  |
| 39  | BR    | 79  | ARG  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | BR    | 83  | TYR  |
| 39  | BR    | 91  | GLN  |
| 39  | BR    | 93  | PHE  |
| 40  | BS    | 6   | LYS  |
| 40  | BS    | 8   | ARG  |
| 40  | BS    | 13  | SER  |
| 40  | BS    | 15  | GLN  |
| 40  | BS    | 16  | LYS  |
| 40  | BS    | 28  | LYS  |
| 40  | BS    | 60  | HIS  |
| 40  | BS    | 67  | ASP  |
| 40  | BS    | 90  | LYS  |
| 40  | BS    | 94  | ASP  |
| 41  | BT    | 1   | MET  |
| 41  | BT    | 4   | GLU  |
| 41  | BT    | 5   | GLU  |
| 41  | BT    | 6   | ARG  |
| 41  | BT    | 8   | LEU  |
| 41  | BT    | 10  | VAL  |
| 41  | BT    | 15  | HIS  |
| 41  | BT    | 26  | LYS  |
| 41  | BT    | 30  | ILE  |
| 41  | BT    | 31  | VAL  |
| 41  | BT    | 44  | LYS  |
| 41  | BT    | 50  | LEU  |
| 41  | BT    | 61  | LEU  |
| 41  | BT    | 68  | LYS  |
| 41  | BT    | 69  | ARG  |
| 41  | BT    | 79  | ASP  |
| 41  | BT    | 85  | VAL  |
| 42  | BU    | 3   | LYS  |
| 42  | BU    | 13  | LEU  |
| 42  | BU    | 25  | LYS  |
| 42  | BU    | 38  | ILE  |
| 42  | BU    | 43  | LYS  |
| 42  | BU    | 48  | VAL  |
| 42  | BU    | 52  | ASN  |
| 42  | BU    | 61  | GLU  |
| 42  | BU    | 64  | ILE  |
| 42  | BU    | 68  | ASN  |
| 42  | BU    | 71  | ILE  |
| 42  | BU    | 72  | PHE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | BU    | 81  | ARG  |
| 42  | BU    | 87  | GLU  |
| 42  | BU    | 90  | LYS  |
| 42  | BU    | 93  | ARG  |
| 42  | BU    | 95  | PHE  |
| 42  | BU    | 98  | ASN  |
| 43  | BW    | 2   | HIS  |
| 43  | BW    | 10  | ARG  |
| 43  | BW    | 18  | LYS  |
| 43  | BW    | 20  | LEU  |
| 43  | BW    | 23  | LYS  |
| 43  | BW    | 40  | ARG  |
| 43  | BW    | 52  | CYS  |
| 43  | BW    | 65  | LYS  |
| 43  | BW    | 69  | GLU  |
| 43  | BW    | 71  | LYS  |
| 43  | BW    | 75  | ASN  |
| 43  | BW    | 81  | ILE  |
| 44  | BX    | 1   | MET  |
| 44  | BX    | 2   | LYS  |
| 44  | BX    | 7   | ARG  |
| 44  | BX    | 12  | GLU  |
| 44  | BX    | 14  | LEU  |
| 44  | BX    | 15  | ASN  |
| 44  | BX    | 17  | GLU  |
| 44  | BX    | 18  | LEU  |
| 44  | BX    | 22  | LEU  |
| 44  | BX    | 24  | GLU  |
| 44  | BX    | 31  | GLN  |
| 44  | BX    | 38  | GLN  |
| 44  | BX    | 45  | GLN  |
| 44  | BX    | 50  | VAL  |
| 44  | BX    | 53  | VAL  |
| 45  | BY    | 6   | ILE  |
| 45  | BY    | 7   | THR  |
| 45  | BY    | 8   | GLN  |
| 45  | BY    | 9   | THR  |
| 45  | BY    | 10  | ARG  |
| 45  | BY    | 15  | ARG  |
| 45  | BY    | 16  | LEU  |
| 45  | BY    | 17  | PRO  |
| 45  | BY    | 31  | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45  | BY    | 37  | ARG  |
| 45  | BY    | 39  | ASP  |
| 46  | BZ    | 1   | MET  |
| 46  | BZ    | 6   | HIS  |
| 46  | BZ    | 8   | LYS  |
| 46  | BZ    | 11  | GLU  |
| 46  | BZ    | 12  | ILE  |
| 46  | BZ    | 13  | THR  |
| 46  | BZ    | 18  | CYS  |
| 46  | BZ    | 24  | ILE  |
| 46  | BZ    | 25  | ARG  |
| 46  | BZ    | 32  | LEU  |
| 46  | BZ    | 33  | ASN  |
| 46  | BZ    | 40  | CYS  |
| 46  | BZ    | 41  | HIS  |
| 46  | BZ    | 44  | PHE  |
| 46  | BZ    | 49  | ARG  |
| 46  | BZ    | 58  | ASP  |
| 46  | BZ    | 70  | LYS  |
| 47  | B0    | 4   | GLN  |
| 47  | B0    | 6   | LYS  |
| 47  | B0    | 8   | THR  |
| 47  | B0    | 14  | MET  |
| 47  | B0    | 25  | THR  |
| 47  | B0    | 27  | LEU  |
| 47  | B0    | 29  | VAL  |
| 47  | B0    | 32  | THR  |
| 47  | B0    | 52  | LYS  |
| 48  | B1    | 5   | ARG  |
| 48  | B1    | 6   | GLU  |
| 48  | B1    | 7   | LYS  |
| 48  | B1    | 8   | ILE  |
| 48  | B1    | 9   | LYS  |
| 48  | B1    | 24  | LYS  |
| 48  | B1    | 32  | LYS  |
| 48  | B1    | 33  | LEU  |
| 48  | B1    | 34  | GLU  |
| 48  | B1    | 36  | LYS  |
| 48  | B1    | 44  | GLN  |
| 48  | B1    | 46  | VAL  |
| 48  | B1    | 49  | LYS  |
| 48  | B1    | 52  | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | B1    | 53  | ILE  |
| 49  | B2    | 18  | PHE  |
| 49  | B2    | 25  | LYS  |
| 49  | B2    | 28  | ARG  |
| 49  | B2    | 29  | GLN  |
| 49  | B2    | 33  | ARG  |
| 50  | B3    | 4   | LYS  |
| 50  | B3    | 6   | VAL  |
| 50  | B3    | 12  | ARG  |
| 50  | B3    | 18  | LYS  |
| 50  | B3    | 21  | PHE  |
| 50  | B3    | 23  | HIS  |
| 50  | B3    | 25  | HIS  |
| 50  | B3    | 29  | ARG  |
| 50  | B3    | 37  | THR  |
| 50  | B3    | 41  | ARG  |
| 50  | B3    | 43  | LEU  |
| 50  | B3    | 44  | ARG  |
| 51  | B4    | 2   | LYS  |
| 51  | B4    | 12  | ARG  |
| 51  | B4    | 19  | ARG  |
| 51  | B4    | 20  | ASP  |
| 51  | B4    | 23  | ILE  |
| 51  | B4    | 32  | LYS  |
| 51  | B4    | 33  | HIS  |
| 51  | B4    | 35  | GLN  |
| 51  | B4    | 37  | GLN  |
| 52  | BI    | 63  | ASP  |
| 2   | CC    | 2   | GLN  |
| 2   | CC    | 13  | ILE  |
| 2   | CC    | 19  | SER  |
| 2   | CC    | 25  | THR  |
| 2   | CC    | 30  | ASP  |
| 2   | CC    | 40  | GLN  |
| 2   | CC    | 46  | LEU  |
| 2   | CC    | 87  | ARG  |
| 2   | CC    | 88  | LYS  |
| 2   | CC    | 96  | VAL  |
| 2   | CC    | 128 | MET  |
| 2   | CC    | 129 | PHE  |
| 2   | CC    | 143 | LEU  |
| 2   | CC    | 164 | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | CC    | 165 | GLU  |
| 2   | CC    | 166 | TRP  |
| 2   | CC    | 168 | ARG  |
| 2   | CC    | 181 | ILE  |
| 2   | CC    | 206 | ILE  |
| 3   | CD    | 2   | ARG  |
| 3   | CD    | 14  | GLU  |
| 3   | CD    | 25  | ARG  |
| 3   | CD    | 28  | ASP  |
| 3   | CD    | 30  | LYS  |
| 3   | CD    | 33  | ILE  |
| 3   | CD    | 39  | GLN  |
| 3   | CD    | 46  | ARG  |
| 3   | CD    | 47  | LEU  |
| 3   | CD    | 49  | ASP  |
| 3   | CD    | 55  | ARG  |
| 3   | CD    | 58  | GLN  |
| 3   | CD    | 84  | ASN  |
| 3   | CD    | 92  | LEU  |
| 3   | CD    | 93  | LEU  |
| 3   | CD    | 100 | VAL  |
| 3   | CD    | 106 | PHE  |
| 3   | CD    | 125 | ASN  |
| 3   | CD    | 127 | ARG  |
| 3   | CD    | 130 | ASN  |
| 3   | CD    | 147 | LYS  |
| 3   | CD    | 154 | VAL  |
| 3   | CD    | 160 | LEU  |
| 3   | CD    | 170 | LEU  |
| 3   | CD    | 186 | GLU  |
| 3   | CD    | 199 | ILE  |
| 4   | CE    | 9   | GLU  |
| 4   | CE    | 11  | GLN  |
| 4   | CE    | 13  | LYS  |
| 4   | CE    | 14  | LEU  |
| 4   | CE    | 23  | THR  |
| 4   | CE    | 25  | LYS  |
| 4   | CE    | 45  | VAL  |
| 4   | CE    | 55  | VAL  |
| 4   | CE    | 61  | LYS  |
| 4   | CE    | 65  | LYS  |
| 4   | CE    | 72  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | CE    | 89  | THR  |
| 4   | CE    | 95  | MET  |
| 4   | CE    | 104 | ILE  |
| 4   | CE    | 120 | HIS  |
| 4   | CE    | 133 | ILE  |
| 4   | CE    | 141 | ASP  |
| 4   | CE    | 144 | GLU  |
| 4   | CE    | 146 | MET  |
| 4   | CE    | 147 | ASN  |
| 4   | CE    | 151 | MET  |
| 5   | CF    | 2   | ARG  |
| 5   | CF    | 3   | HIS  |
| 5   | CF    | 6   | ILE  |
| 5   | CF    | 13  | ASP  |
| 5   | CF    | 39  | LEU  |
| 5   | CF    | 54  | LEU  |
| 5   | CF    | 55  | HIS  |
| 5   | CF    | 59  | TYR  |
| 5   | CF    | 74  | LEU  |
| 5   | CF    | 76  | THR  |
| 5   | CF    | 86  | ARG  |
| 5   | CF    | 91  | ARG  |
| 6   | CG    | 2   | ARG  |
| 6   | CG    | 8   | GLN  |
| 6   | CG    | 11  | ILE  |
| 6   | CG    | 12  | LEU  |
| 6   | CG    | 26  | VAL  |
| 6   | CG    | 46  | LEU  |
| 6   | CG    | 75  | LYS  |
| 6   | CG    | 84  | TYR  |
| 6   | CG    | 89  | GLU  |
| 6   | CG    | 98  | LEU  |
| 6   | CG    | 109 | LYS  |
| 6   | CG    | 115 | MET  |
| 6   | CG    | 117 | LEU  |
| 7   | CH    | 2   | MET  |
| 7   | CH    | 6   | ILE  |
| 7   | CH    | 8   | ASP  |
| 7   | CH    | 55  | LYS  |
| 7   | CH    | 57  | GLU  |
| 7   | CH    | 68  | LYS  |
| 7   | CH    | 72  | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | CH    | 82  | LEU  |
| 7   | CH    | 88  | LYS  |
| 7   | CH    | 93  | LYS  |
| 7   | CH    | 100 | ILE  |
| 7   | CH    | 107 | LYS  |
| 7   | CH    | 123 | GLU  |
| 7   | CH    | 124 | ILE  |
| 8   | CI    | 19  | PHE  |
| 8   | CI    | 26  | LYS  |
| 8   | CI    | 27  | ILE  |
| 8   | CI    | 31  | GLN  |
| 8   | CI    | 45  | MET  |
| 8   | CI    | 60  | LEU  |
| 8   | CI    | 61  | ASP  |
| 8   | CI    | 62  | LEU  |
| 8   | CI    | 83  | THR  |
| 8   | CI    | 87  | MET  |
| 8   | CI    | 109 | GLN  |
| 8   | CI    | 126 | PHE  |
| 9   | CJ    | 17  | LEU  |
| 9   | CJ    | 32  | THR  |
| 9   | CJ    | 37  | ARG  |
| 9   | CJ    | 47  | GLU  |
| 9   | CJ    | 71  | LEU  |
| 9   | CJ    | 77  | VAL  |
| 9   | CJ    | 78  | GLU  |
| 9   | CJ    | 99  | GLN  |
| 10  | CK    | 31  | VAL  |
| 10  | CK    | 34  | THR  |
| 10  | CK    | 64  | VAL  |
| 10  | CK    | 75  | GLU  |
| 10  | CK    | 76  | TYR  |
| 10  | CK    | 78  | ILE  |
| 10  | CK    | 84  | MET  |
| 10  | CK    | 94  | SER  |
| 10  | CK    | 97  | ARG  |
| 10  | CK    | 109 | ILE  |
| 10  | CK    | 115 | ILE  |
| 11  | CL    | 4   | ASN  |
| 11  | CL    | 7   | VAL  |
| 11  | CL    | 8   | ARG  |
| 11  | CL    | 14  | LYS  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | CL    | 17  | LYS  |
| 11  | CL    | 26  | CYS  |
| 11  | CL    | 28  | GLN  |
| 11  | CL    | 34  | THR  |
| 11  | CL    | 40  | THR  |
| 11  | CL    | 49  | ARG  |
| 11  | CL    | 54  | VAL  |
| 11  | CL    | 61  | GLU  |
| 11  | CL    | 69  | GLU  |
| 11  | CL    | 75  | GLU  |
| 11  | CL    | 88  | ASP  |
| 11  | CL    | 93  | ARG  |
| 11  | CL    | 107 | LYS  |
| 11  | CL    | 111 | GLN  |
| 11  | CL    | 120 | ARG  |
| 11  | CL    | 122 | LYS  |
| 12  | CM    | 2   | ARG  |
| 12  | CM    | 15  | VAL  |
| 12  | CM    | 40  | GLU  |
| 12  | CM    | 49  | GLU  |
| 12  | CM    | 56  | ARG  |
| 12  | CM    | 67  | ASP  |
| 12  | CM    | 92  | ARG  |
| 12  | CM    | 102 | LYS  |
| 12  | CM    | 106 | ARG  |
| 12  | CM    | 109 | LYS  |
| 12  | CM    | 112 | ARG  |
| 13  | CN    | 2   | LYS  |
| 13  | CN    | 3   | GLN  |
| 13  | CN    | 5   | MET  |
| 13  | CN    | 11  | LYS  |
| 13  | CN    | 44  | VAL  |
| 13  | CN    | 48  | GLN  |
| 13  | CN    | 50  | LEU  |
| 13  | CN    | 72  | PHE  |
| 13  | CN    | 82  | LYS  |
| 13  | CN    | 89  | ARG  |
| 13  | CN    | 95  | LEU  |
| 14  | CO    | 4   | THR  |
| 14  | CO    | 19  | ASN  |
| 14  | CO    | 39  | GLN  |
| 14  | CO    | 44  | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | CO    | 56  | LEU  |
| 14  | CO    | 59  | VAL  |
| 14  | CO    | 63  | ARG  |
| 14  | CO    | 69  | LEU  |
| 14  | CO    | 78  | THR  |
| 14  | CO    | 83  | ARG  |
| 15  | CP    | 5   | ARG  |
| 15  | CP    | 19  | VAL  |
| 15  | CP    | 28  | ARG  |
| 15  | CP    | 32  | PHE  |
| 15  | CP    | 35  | ARG  |
| 15  | CP    | 50  | THR  |
| 15  | CP    | 57  | ILE  |
| 15  | CP    | 67  | ILE  |
| 16  | CQ    | 20  | ILE  |
| 16  | CQ    | 29  | LYS  |
| 16  | CQ    | 39  | ARG  |
| 16  | CQ    | 60  | ILE  |
| 16  | CQ    | 66  | LEU  |
| 16  | CQ    | 73  | THR  |
| 16  | CQ    | 74  | LEU  |
| 16  | CQ    | 80  | LYS  |
| 17  | CR    | 25  | ILE  |
| 17  | CR    | 34  | GLU  |
| 17  | CR    | 38  | ILE  |
| 17  | CR    | 42  | ARG  |
| 17  | CR    | 47  | ARG  |
| 18  | CS    | 5   | LYS  |
| 18  | CS    | 10  | ILE  |
| 18  | CS    | 12  | LEU  |
| 18  | CS    | 13  | HIS  |
| 18  | CS    | 26  | ASP  |
| 18  | CS    | 27  | LYS  |
| 18  | CS    | 28  | LYS  |
| 18  | CS    | 36  | ARG  |
| 18  | CS    | 47  | THR  |
| 18  | CS    | 64  | GLU  |
| 18  | CS    | 73  | PHE  |
| 18  | CS    | 78  | THR  |
| 19  | CT    | 11  | ILE  |
| 19  | CT    | 29  | THR  |
| 19  | CT    | 35  | TYR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | CT    | 47  | GLN  |
| 19  | CT    | 51  | ASN  |
| 19  | CT    | 53  | MET  |
| 19  | CT    | 63  | LYS  |
| 19  | CT    | 66  | ILE  |
| 19  | CT    | 69  | ASN  |
| 19  | CT    | 70  | LYS  |
| 19  | CT    | 77  | ASN  |
| 20  | CB    | 8   | MET  |
| 20  | CB    | 15  | PHE  |
| 20  | CB    | 35  | ASN  |
| 20  | CB    | 36  | LYS  |
| 20  | CB    | 37  | VAL  |
| 20  | CB    | 46  | VAL  |
| 20  | CB    | 53  | LEU  |
| 20  | CB    | 57  | ASN  |
| 20  | CB    | 62  | ARG  |
| 20  | CB    | 84  | LEU  |
| 20  | CB    | 94  | ARG  |
| 20  | CB    | 104 | LYS  |
| 20  | CB    | 116 | LEU  |
| 20  | CB    | 121 | GLN  |
| 20  | CB    | 127 | LYS  |
| 20  | CB    | 132 | GLU  |
| 20  | CB    | 139 | GLU  |
| 20  | CB    | 143 | LEU  |
| 20  | CB    | 145 | ASN  |
| 20  | CB    | 176 | ASN  |
| 20  | CB    | 188 | THR  |
| 20  | CB    | 191 | ASP  |
| 20  | CB    | 207 | ARG  |
| 20  | CB    | 213 | LEU  |
| 20  | CB    | 222 | GLU  |
| 21  | CU    | 7   | GLU  |
| 21  | CU    | 8   | ASN  |
| 21  | CU    | 20  | ARG  |
| 21  | CU    | 24  | LYS  |
| 21  | CU    | 33  | ARG  |
| 21  | CU    | 35  | GLU  |
| 21  | CU    | 36  | PHE  |
| 21  | CU    | 38  | GLU  |
| 21  | CU    | 42  | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | DV    | 35  | GLU  |
| 24  | DV    | 48  | MET  |
| 24  | DV    | 51  | GLN  |
| 24  | DV    | 53  | LYS  |
| 24  | DV    | 69  | GLU  |
| 24  | DV    | 70  | ILE  |
| 24  | DV    | 86  | LEU  |
| 25  | DC    | 12  | ARG  |
| 25  | DC    | 28  | PRO  |
| 25  | DC    | 29  | PHE  |
| 25  | DC    | 32  | LEU  |
| 25  | DC    | 33  | LEU  |
| 25  | DC    | 38  | LYS  |
| 25  | DC    | 42  | ARG  |
| 25  | DC    | 47  | ARG  |
| 25  | DC    | 49  | THR  |
| 25  | DC    | 50  | THR  |
| 25  | DC    | 51  | ARG  |
| 25  | DC    | 57  | HIS  |
| 25  | DC    | 58  | LYS  |
| 25  | DC    | 62  | ARG  |
| 25  | DC    | 69  | ASN  |
| 25  | DC    | 70  | LYS  |
| 25  | DC    | 78  | GLU  |
| 25  | DC    | 85  | ASN  |
| 25  | DC    | 102 | TYR  |
| 25  | DC    | 104 | LEU  |
| 25  | DC    | 107 | LYS  |
| 25  | DC    | 109 | LEU  |
| 25  | DC    | 110 | LYS  |
| 25  | DC    | 125 | PRO  |
| 25  | DC    | 127 | ASN  |
| 25  | DC    | 129 | LEU  |
| 25  | DC    | 133 | ASN  |
| 25  | DC    | 141 | HIS  |
| 25  | DC    | 143 | VAL  |
| 25  | DC    | 145 | MET  |
| 25  | DC    | 152 | GLN  |
| 25  | DC    | 155 | ARG  |
| 25  | DC    | 164 | VAL  |
| 25  | DC    | 171 | VAL  |
| 25  | DC    | 172 | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | DC    | 180 | MET  |
| 25  | DC    | 194 | VAL  |
| 25  | DC    | 201 | LEU  |
| 25  | DC    | 203 | VAL  |
| 25  | DC    | 206 | LYS  |
| 25  | DC    | 211 | ARG  |
| 25  | DC    | 220 | ARG  |
| 25  | DC    | 231 | HIS  |
| 25  | DC    | 235 | GLU  |
| 25  | DC    | 237 | ARG  |
| 25  | DC    | 246 | PRO  |
| 25  | DC    | 250 | GLN  |
| 25  | DC    | 251 | THR  |
| 25  | DC    | 254 | LYS  |
| 25  | DC    | 265 | PHE  |
| 26  | DD    | 1   | MET  |
| 26  | DD    | 4   | LEU  |
| 26  | DD    | 7   | LYS  |
| 26  | DD    | 9   | VAL  |
| 26  | DD    | 14  | ILE  |
| 26  | DD    | 15  | PHE  |
| 26  | DD    | 17  | GLU  |
| 26  | DD    | 22  | ILE  |
| 26  | DD    | 27  | ILE  |
| 26  | DD    | 33  | ARG  |
| 26  | DD    | 34  | VAL  |
| 26  | DD    | 36  | GLN  |
| 26  | DD    | 40  | LEU  |
| 26  | DD    | 56  | LYS  |
| 26  | DD    | 60  | VAL  |
| 26  | DD    | 70  | LYS  |
| 26  | DD    | 79  | LEU  |
| 26  | DD    | 82  | PHE  |
| 26  | DD    | 88  | GLU  |
| 26  | DD    | 92  | VAL  |
| 26  | DD    | 104 | VAL  |
| 26  | DD    | 106 | LYS  |
| 26  | DD    | 114 | LYS  |
| 26  | DD    | 121 | THR  |
| 26  | DD    | 124 | ARG  |
| 26  | DD    | 127 | PHE  |
| 26  | DD    | 133 | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | DD    | 138 | LEU  |
| 26  | DD    | 139 | SER  |
| 26  | DD    | 142 | VAL  |
| 26  | DD    | 146 | ILE  |
| 26  | DD    | 151 | THR  |
| 26  | DD    | 152 | PRO  |
| 26  | DD    | 160 | LYS  |
| 26  | DD    | 176 | ASP  |
| 26  | DD    | 185 | ASN  |
| 26  | DD    | 188 | LEU  |
| 26  | DD    | 202 | ILE  |
| 27  | DE    | 1   | MET  |
| 27  | DE    | 33  | VAL  |
| 27  | DE    | 43  | THR  |
| 27  | DE    | 49  | ARG  |
| 27  | DE    | 84  | THR  |
| 27  | DE    | 99  | LYS  |
| 27  | DE    | 100 | MET  |
| 27  | DE    | 109 | LEU  |
| 27  | DE    | 111 | GLU  |
| 27  | DE    | 115 | GLN  |
| 27  | DE    | 117 | ARG  |
| 27  | DE    | 130 | LYS  |
| 27  | DE    | 133 | LEU  |
| 27  | DE    | 134 | LEU  |
| 27  | DE    | 137 | LYS  |
| 27  | DE    | 138 | LEU  |
| 27  | DE    | 143 | LEU  |
| 27  | DE    | 147 | LEU  |
| 27  | DE    | 148 | ILE  |
| 27  | DE    | 164 | LEU  |
| 27  | DE    | 165 | HIS  |
| 27  | DE    | 167 | VAL  |
| 27  | DE    | 173 | THR  |
| 27  | DE    | 184 | ASP  |
| 27  | DE    | 185 | LYS  |
| 27  | DE    | 188 | MET  |
| 27  | DE    | 194 | LYS  |
| 28  | DF    | 16  | MET  |
| 28  | DF    | 45  | ASP  |
| 28  | DF    | 56  | LEU  |
| 28  | DF    | 59  | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | DF    | 71  | LYS  |
| 28  | DF    | 76  | PHE  |
| 28  | DF    | 84  | ILE  |
| 28  | DF    | 86  | CYS  |
| 28  | DF    | 90  | LEU  |
| 28  | DF    | 95  | MET  |
| 28  | DF    | 103 | ILE  |
| 28  | DF    | 105 | ILE  |
| 28  | DF    | 107 | VAL  |
| 28  | DF    | 132 | ARG  |
| 28  | DF    | 133 | GLU  |
| 28  | DF    | 134 | GLN  |
| 28  | DF    | 135 | ILE  |
| 28  | DF    | 141 | ASP  |
| 28  | DF    | 143 | ASP  |
| 28  | DF    | 149 | ARG  |
| 28  | DF    | 161 | SER  |
| 28  | DF    | 164 | GLU  |
| 28  | DF    | 177 | ARG  |
| 29  | DG    | 8   | VAL  |
| 29  | DG    | 15  | ASP  |
| 29  | DG    | 16  | VAL  |
| 29  | DG    | 17  | LYS  |
| 29  | DG    | 25  | ILE  |
| 29  | DG    | 29  | ASN  |
| 29  | DG    | 31  | GLU  |
| 29  | DG    | 35  | THR  |
| 29  | DG    | 43  | LYS  |
| 29  | DG    | 71  | LEU  |
| 29  | DG    | 85  | LYS  |
| 29  | DG    | 86  | LEU  |
| 29  | DG    | 104 | LEU  |
| 29  | DG    | 113 | ASP  |
| 29  | DG    | 116 | LEU  |
| 29  | DG    | 121 | THR  |
| 29  | DG    | 123 | GLU  |
| 29  | DG    | 151 | ARG  |
| 29  | DG    | 154 | GLU  |
| 29  | DG    | 161 | VAL  |
| 29  | DG    | 171 | LYS  |
| 29  | DG    | 174 | LYS  |
| 30  | DH    | 4   | ILE  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | DH    | 8   | LYS  |
| 30  | DH    | 11  | ASN  |
| 30  | DH    | 30  | LEU  |
| 30  | DH    | 38  | PRO  |
| 30  | DH    | 45  | GLU  |
| 30  | DH    | 53  | GLU  |
| 30  | DH    | 57  | LYS  |
| 30  | DH    | 68  | ARG  |
| 30  | DH    | 70  | GLU  |
| 30  | DH    | 75  | LEU  |
| 30  | DH    | 76  | GLU  |
| 30  | DH    | 96  | THR  |
| 30  | DH    | 97  | ARG  |
| 30  | DH    | 119 | ASN  |
| 30  | DH    | 124 | THR  |
| 30  | DH    | 129 | GLU  |
| 30  | DH    | 137 | GLU  |
| 30  | DH    | 141 | LYS  |
| 31  | DJ    | 1   | MET  |
| 31  | DJ    | 3   | THR  |
| 31  | DJ    | 7   | LYS  |
| 31  | DJ    | 15  | TRP  |
| 31  | DJ    | 25  | LEU  |
| 31  | DJ    | 27  | ARG  |
| 31  | DJ    | 28  | LEU  |
| 31  | DJ    | 31  | GLU  |
| 31  | DJ    | 36  | LEU  |
| 31  | DJ    | 41  | LYS  |
| 31  | DJ    | 45  | THR  |
| 31  | DJ    | 47  | HIS  |
| 31  | DJ    | 57  | LEU  |
| 31  | DJ    | 61  | LYS  |
| 31  | DJ    | 69  | ARG  |
| 31  | DJ    | 85  | LYS  |
| 31  | DJ    | 91  | GLU  |
| 31  | DJ    | 95  | ARG  |
| 31  | DJ    | 118 | MET  |
| 31  | DJ    | 121 | LYS  |
| 31  | DJ    | 132 | HIS  |
| 31  | DJ    | 135 | GLN  |
| 31  | DJ    | 140 | LEU  |
| 32  | DK    | 2   | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | DK    | 8   | LEU  |
| 32  | DK    | 10  | VAL  |
| 32  | DK    | 32  | TYR  |
| 32  | DK    | 37  | ASP  |
| 32  | DK    | 58  | LEU  |
| 32  | DK    | 65  | THR  |
| 32  | DK    | 79  | PHE  |
| 32  | DK    | 98  | ARG  |
| 32  | DK    | 104 | THR  |
| 32  | DK    | 105 | ARG  |
| 32  | DK    | 120 | PRO  |
| 33  | DL    | 2   | ARG  |
| 33  | DL    | 4   | ASN  |
| 33  | DL    | 14  | LYS  |
| 33  | DL    | 17  | LYS  |
| 33  | DL    | 19  | LEU  |
| 33  | DL    | 21  | ARG  |
| 33  | DL    | 25  | SER  |
| 33  | DL    | 38  | GLN  |
| 33  | DL    | 39  | LYS  |
| 33  | DL    | 46  | VAL  |
| 33  | DL    | 48  | ARG  |
| 33  | DL    | 54  | GLN  |
| 33  | DL    | 55  | MET  |
| 33  | DL    | 57  | LEU  |
| 33  | DL    | 60  | ARG  |
| 33  | DL    | 69  | ARG  |
| 33  | DL    | 77  | ILE  |
| 33  | DL    | 92  | LEU  |
| 33  | DL    | 96  | LYS  |
| 33  | DL    | 104 | GLN  |
| 33  | DL    | 106 | GLU  |
| 33  | DL    | 107 | PHE  |
| 33  | DL    | 109 | LYS  |
| 33  | DL    | 111 | ILE  |
| 33  | DL    | 115 | GLU  |
| 33  | DL    | 116 | VAL  |
| 33  | DL    | 119 | PRO  |
| 33  | DL    | 125 | LEU  |
| 33  | DL    | 127 | VAL  |
| 33  | DL    | 128 | THR  |
| 33  | DL    | 135 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | DL    | 136 | GLU  |
| 33  | DL    | 141 | LYS  |
| 33  | DL    | 144 | GLU  |
| 34  | DM    | 1   | MET  |
| 34  | DM    | 5   | LYS  |
| 34  | DM    | 9   | PHE  |
| 34  | DM    | 14  | LYS  |
| 34  | DM    | 16  | ARG  |
| 34  | DM    | 22  | GLN  |
| 34  | DM    | 26  | VAL  |
| 34  | DM    | 33  | LEU  |
| 34  | DM    | 42  | THR  |
| 34  | DM    | 54  | THR  |
| 34  | DM    | 71  | LYS  |
| 34  | DM    | 72  | PRO  |
| 34  | DM    | 76  | LYS  |
| 34  | DM    | 80  | VAL  |
| 34  | DM    | 81  | ARG  |
| 34  | DM    | 84  | LYS  |
| 34  | DM    | 88  | ASN  |
| 34  | DM    | 90  | GLU  |
| 34  | DM    | 91  | TYR  |
| 34  | DM    | 93  | VAL  |
| 34  | DM    | 96  | ILE  |
| 34  | DM    | 100 | LYS  |
| 34  | DM    | 101 | VAL  |
| 34  | DM    | 105 | MET  |
| 34  | DM    | 106 | ASP  |
| 34  | DM    | 111 | GLU  |
| 34  | DM    | 115 | GLU  |
| 34  | DM    | 118 | LYS  |
| 34  | DM    | 123 | LYS  |
| 34  | DM    | 124 | LEU  |
| 34  | DM    | 127 | LYS  |
| 35  | DN    | 2   | ARG  |
| 35  | DN    | 4   | ARG  |
| 35  | DN    | 5   | LYS  |
| 35  | DN    | 12  | ARG  |
| 35  | DN    | 18  | GLN  |
| 35  | DN    | 36  | THR  |
| 35  | DN    | 42  | LYS  |
| 35  | DN    | 49  | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | DN    | 52  | ILE  |
| 35  | DN    | 57  | THR  |
| 35  | DN    | 70  | THR  |
| 35  | DN    | 71  | ARG  |
| 35  | DN    | 79  | LEU  |
| 35  | DN    | 81  | ASN  |
| 35  | DN    | 87  | PHE  |
| 35  | DN    | 96  | ARG  |
| 35  | DN    | 99  | LYS  |
| 35  | DN    | 117 | ASP  |
| 35  | DN    | 121 | LYS  |
| 36  | DO    | 12  | THR  |
| 36  | DO    | 18  | LEU  |
| 36  | DO    | 21  | LEU  |
| 36  | DO    | 27  | VAL  |
| 36  | DO    | 40  | ILE  |
| 36  | DO    | 60  | GLU  |
| 36  | DO    | 65  | THR  |
| 36  | DO    | 68  | LYS  |
| 36  | DO    | 84  | GLU  |
| 36  | DO    | 87  | ILE  |
| 36  | DO    | 98  | GLN  |
| 36  | DO    | 100 | HIS  |
| 37  | DP    | 5   | LYS  |
| 37  | DP    | 8   | GLU  |
| 37  | DP    | 10  | GLU  |
| 37  | DP    | 13  | LYS  |
| 37  | DP    | 18  | SER  |
| 37  | DP    | 19  | PHE  |
| 37  | DP    | 23  | ASP  |
| 37  | DP    | 24  | THR  |
| 37  | DP    | 27  | VAL  |
| 37  | DP    | 37  | LYS  |
| 37  | DP    | 47  | ILE  |
| 37  | DP    | 50  | ARG  |
| 37  | DP    | 54  | LEU  |
| 37  | DP    | 60  | VAL  |
| 37  | DP    | 61  | ARG  |
| 37  | DP    | 70  | GLU  |
| 37  | DP    | 71  | ARG  |
| 37  | DP    | 73  | PHE  |
| 37  | DP    | 74  | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | DP    | 76  | HIS  |
| 37  | DP    | 80  | VAL  |
| 37  | DP    | 81  | ASP  |
| 37  | DP    | 84  | SER  |
| 37  | DP    | 87  | ARG  |
| 37  | DP    | 100 | ARG  |
| 37  | DP    | 101 | GLU  |
| 37  | DP    | 108 | ARG  |
| 37  | DP    | 109 | ILE  |
| 37  | DP    | 111 | GLU  |
| 37  | DP    | 113 | LEU  |
| 38  | DQ    | 4   | LYS  |
| 38  | DQ    | 13  | HIS  |
| 38  | DQ    | 17  | LEU  |
| 38  | DQ    | 36  | GLN  |
| 38  | DQ    | 39  | ILE  |
| 38  | DQ    | 40  | LYS  |
| 38  | DQ    | 50  | ARG  |
| 38  | DQ    | 52  | ARG  |
| 38  | DQ    | 53  | LYS  |
| 38  | DQ    | 58  | GLN  |
| 38  | DQ    | 63  | ARG  |
| 38  | DQ    | 70  | GLN  |
| 38  | DQ    | 84  | LYS  |
| 38  | DQ    | 90  | ASP  |
| 38  | DQ    | 93  | ILE  |
| 38  | DQ    | 100 | PHE  |
| 38  | DQ    | 103 | VAL  |
| 39  | DR    | 4   | VAL  |
| 39  | DR    | 6   | GLN  |
| 39  | DR    | 7   | SER  |
| 39  | DR    | 14  | VAL  |
| 39  | DR    | 18  | GLN  |
| 39  | DR    | 19  | THR  |
| 39  | DR    | 22  | LEU  |
| 39  | DR    | 23  | GLU  |
| 39  | DR    | 26  | ASP  |
| 39  | DR    | 32  | THR  |
| 39  | DR    | 43  | ASN  |
| 39  | DR    | 62  | GLU  |
| 39  | DR    | 75  | VAL  |
| 39  | DR    | 84  | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | DR    | 91  | GLN  |
| 39  | DR    | 99  | THR  |
| 39  | DR    | 102 | SER  |
| 40  | DS    | 7   | HIS  |
| 40  | DS    | 23  | LEU  |
| 40  | DS    | 24  | ILE  |
| 40  | DS    | 25  | ARG  |
| 40  | DS    | 27  | LYS  |
| 40  | DS    | 46  | LEU  |
| 40  | DS    | 55  | ILE  |
| 40  | DS    | 73  | LYS  |
| 40  | DS    | 82  | MET  |
| 40  | DS    | 83  | LYS  |
| 40  | DS    | 85  | ILE  |
| 40  | DS    | 105 | VAL  |
| 40  | DS    | 107 | VAL  |
| 41  | DT    | 3   | ARG  |
| 41  | DT    | 5   | GLU  |
| 41  | DT    | 11  | LEU  |
| 41  | DT    | 22  | THR  |
| 41  | DT    | 24  | MET  |
| 41  | DT    | 33  | LYS  |
| 41  | DT    | 57  | VAL  |
| 41  | DT    | 58  | VAL  |
| 41  | DT    | 64  | LYS  |
| 41  | DT    | 66  | LYS  |
| 41  | DT    | 68  | LYS  |
| 41  | DT    | 73  | ARG  |
| 41  | DT    | 76  | ARG  |
| 41  | DT    | 88  | LYS  |
| 42  | DU    | 4   | ILE  |
| 42  | DU    | 8   | ASP  |
| 42  | DU    | 13  | LEU  |
| 42  | DU    | 27  | VAL  |
| 42  | DU    | 28  | LEU  |
| 42  | DU    | 40  | LEU  |
| 42  | DU    | 42  | LYS  |
| 42  | DU    | 43  | LYS  |
| 42  | DU    | 52  | ASN  |
| 42  | DU    | 57  | ILE  |
| 42  | DU    | 60  | LYS  |
| 42  | DU    | 65  | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | DU    | 71  | ILE  |
| 42  | DU    | 73  | ASN  |
| 42  | DU    | 85  | ARG  |
| 42  | DU    | 88  | ASP  |
| 42  | DU    | 90  | LYS  |
| 42  | DU    | 92  | VAL  |
| 42  | DU    | 96  | LYS  |
| 43  | DW    | 2   | HIS  |
| 43  | DW    | 3   | LYS  |
| 43  | DW    | 4   | LYS  |
| 43  | DW    | 13  | ARG  |
| 43  | DW    | 18  | LYS  |
| 43  | DW    | 19  | ARG  |
| 43  | DW    | 20  | LEU  |
| 43  | DW    | 37  | VAL  |
| 43  | DW    | 50  | VAL  |
| 43  | DW    | 65  | LYS  |
| 43  | DW    | 75  | ASN  |
| 43  | DW    | 82  | GLU  |
| 43  | DW    | 84  | GLU  |
| 44  | DX    | 8   | GLU  |
| 44  | DX    | 9   | LYS  |
| 44  | DX    | 17  | GLU  |
| 44  | DX    | 18  | LEU  |
| 44  | DX    | 25  | GLN  |
| 44  | DX    | 28  | LEU  |
| 44  | DX    | 30  | MET  |
| 44  | DX    | 36  | GLN  |
| 44  | DX    | 39  | GLN  |
| 44  | DX    | 47  | ARG  |
| 45  | DY    | 5   | LYS  |
| 45  | DY    | 10  | ARG  |
| 45  | DY    | 13  | ILE  |
| 45  | DY    | 23  | LEU  |
| 45  | DY    | 26  | LEU  |
| 45  | DY    | 35  | VAL  |
| 45  | DY    | 40  | THR  |
| 45  | DY    | 43  | ILE  |
| 45  | DY    | 53  | MET  |
| 45  | DY    | 57  | GLU  |
| 46  | DZ    | 10  | GLU  |
| 46  | DZ    | 12  | ILE  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | DZ    | 20  | ASN  |
| 46  | DZ    | 24  | ILE  |
| 46  | DZ    | 28  | VAL  |
| 46  | DZ    | 31  | ASP  |
| 46  | DZ    | 34  | LEU  |
| 46  | DZ    | 50  | ASP  |
| 47  | D0    | 2   | VAL  |
| 47  | D0    | 5   | ASN  |
| 47  | D0    | 9   | ARG  |
| 47  | D0    | 15  | ARG  |
| 47  | D0    | 19  | ASP  |
| 47  | D0    | 21  | LEU  |
| 47  | D0    | 22  | THR  |
| 47  | D0    | 52  | LYS  |
| 47  | D0    | 53  | VAL  |
| 48  | D1    | 8   | ILE  |
| 48  | D1    | 18  | HIS  |
| 48  | D1    | 19  | PHE  |
| 48  | D1    | 22  | THR  |
| 48  | D1    | 24  | LYS  |
| 48  | D1    | 26  | LYS  |
| 48  | D1    | 27  | ARG  |
| 48  | D1    | 35  | LEU  |
| 48  | D1    | 44  | GLN  |
| 48  | D1    | 49  | LYS  |
| 49  | D2    | 10  | LEU  |
| 49  | D2    | 18  | PHE  |
| 49  | D2    | 19  | ARG  |
| 49  | D2    | 25  | LYS  |
| 49  | D2    | 28  | ARG  |
| 49  | D2    | 34  | ARG  |
| 49  | D2    | 39  | ARG  |
| 49  | D2    | 44  | VAL  |
| 49  | D2    | 46  | LYS  |
| 50  | D3    | 2   | LYS  |
| 50  | D3    | 6   | VAL  |
| 50  | D3    | 7   | ARG  |
| 50  | D3    | 24  | LYS  |
| 50  | D3    | 29  | ARG  |
| 50  | D3    | 32  | LEU  |
| 50  | D3    | 34  | LYS  |
| 50  | D3    | 51  | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | D3    | 54  | LEU  |
| 50  | D3    | 61  | LEU  |
| 51  | D4    | 1   | MET  |
| 51  | D4    | 2   | LYS  |
| 51  | D4    | 17  | VAL  |
| 51  | D4    | 18  | LYS  |
| 51  | D4    | 19  | ARG  |
| 51  | D4    | 23  | ILE  |
| 51  | D4    | 24  | ARG  |
| 51  | D4    | 25  | VAL  |
| 51  | D4    | 26  | ILE  |
| 51  | D4    | 30  | GLU  |
| 51  | D4    | 31  | PRO  |
| 51  | D4    | 35  | GLN  |
| 51  | D4    | 36  | ARG  |
| 52  | DI    | 2   | LYS  |
| 52  | DI    | 36  | GLU  |
| 52  | DI    | 54  | ILE  |
| 52  | DI    | 121 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (349) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AC    | 2   | GLN  |
| 2   | AC    | 5   | HIS  |
| 2   | AC    | 40  | GLN  |
| 2   | AC    | 68  | HIS  |
| 2   | AC    | 122 | GLN  |
| 2   | AC    | 139 | ASN  |
| 2   | AC    | 184 | ASN  |
| 3   | AD    | 73  | ASN  |
| 3   | AD    | 84  | ASN  |
| 3   | AD    | 99  | ASN  |
| 3   | AD    | 115 | GLN  |
| 3   | AD    | 135 | GLN  |
| 3   | AD    | 151 | GLN  |
| 3   | AD    | 195 | ASN  |
| 4   | AE    | 69  | ASN  |
| 4   | AE    | 72  | ASN  |
| 4   | AE    | 81  | GLN  |
| 4   | AE    | 120 | HIS  |
| 4   | AE    | 121 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | AE    | 131 | ASN  |
| 4   | AE    | 134 | ASN  |
| 4   | AE    | 147 | ASN  |
| 5   | AF    | 14  | GLN  |
| 5   | AF    | 17  | GLN  |
| 5   | AF    | 46  | GLN  |
| 5   | AF    | 58  | HIS  |
| 6   | AG    | 67  | ASN  |
| 6   | AG    | 85  | GLN  |
| 6   | AG    | 121 | ASN  |
| 7   | AH    | 3   | GLN  |
| 7   | AH    | 17  | GLN  |
| 7   | AH    | 37  | ASN  |
| 7   | AH    | 75  | GLN  |
| 7   | AH    | 117 | GLN  |
| 8   | AI    | 4   | GLN  |
| 8   | AI    | 24  | ASN  |
| 8   | AI    | 30  | ASN  |
| 8   | AI    | 31  | GLN  |
| 8   | AI    | 36  | GLN  |
| 8   | AI    | 49  | GLN  |
| 8   | AI    | 109 | GLN  |
| 9   | AJ    | 15  | HIS  |
| 9   | AJ    | 20  | GLN  |
| 9   | AJ    | 35  | GLN  |
| 9   | AJ    | 99  | GLN  |
| 10  | AK    | 14  | GLN  |
| 10  | AK    | 37  | GLN  |
| 10  | AK    | 118 | ASN  |
| 11  | AL    | 28  | GLN  |
| 11  | AL    | 58  | ASN  |
| 13  | AN    | 59  | GLN  |
| 13  | AN    | 61  | ASN  |
| 13  | AN    | 65  | GLN  |
| 14  | AO    | 27  | GLN  |
| 14  | AO    | 34  | GLN  |
| 14  | AO    | 36  | ASN  |
| 14  | AO    | 39  | GLN  |
| 15  | AP    | 9   | HIS  |
| 15  | AP    | 29  | ASN  |
| 15  | AP    | 63  | GLN  |
| 17  | AR    | 53  | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | AS    | 13  | HIS  |
| 18  | AS    | 55  | GLN  |
| 18  | AS    | 56  | HIS  |
| 19  | AT    | 12  | GLN  |
| 19  | AT    | 20  | ASN  |
| 19  | AT    | 54  | GLN  |
| 19  | AT    | 60  | GLN  |
| 20  | AB    | 17  | HIS  |
| 20  | AB    | 23  | ASN  |
| 20  | AB    | 35  | ASN  |
| 20  | AB    | 41  | ASN  |
| 20  | AB    | 108 | GLN  |
| 20  | AB    | 119 | GLN  |
| 20  | AB    | 121 | GLN  |
| 20  | AB    | 145 | ASN  |
| 20  | AB    | 167 | HIS  |
| 20  | AB    | 202 | ASN  |
| 24  | BV    | 51  | GLN  |
| 24  | BV    | 80  | HIS  |
| 24  | BV    | 88  | HIS  |
| 25  | BC    | 14  | HIS  |
| 25  | BC    | 24  | HIS  |
| 25  | BC    | 36  | ASN  |
| 25  | BC    | 52  | HIS  |
| 25  | BC    | 89  | ASN  |
| 25  | BC    | 127 | ASN  |
| 25  | BC    | 133 | ASN  |
| 25  | BC    | 162 | GLN  |
| 25  | BC    | 225 | ASN  |
| 25  | BC    | 238 | ASN  |
| 25  | BC    | 250 | GLN  |
| 26  | BD    | 32  | ASN  |
| 26  | BD    | 49  | GLN  |
| 26  | BD    | 134 | HIS  |
| 26  | BD    | 148 | GLN  |
| 26  | BD    | 167 | ASN  |
| 26  | BD    | 173 | GLN  |
| 26  | BD    | 185 | ASN  |
| 27  | BE    | 92  | HIS  |
| 27  | BE    | 94  | GLN  |
| 27  | BE    | 136 | GLN  |
| 27  | BE    | 156 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | BE    | 195 | GLN  |
| 28  | BF    | 26  | GLN  |
| 28  | BF    | 126 | ASN  |
| 29  | BG    | 19  | ASN  |
| 29  | BG    | 21  | GLN  |
| 29  | BG    | 29  | ASN  |
| 29  | BG    | 37  | ASN  |
| 29  | BG    | 63  | GLN  |
| 29  | BG    | 138 | GLN  |
| 30  | BH    | 2   | GLN  |
| 30  | BH    | 11  | ASN  |
| 30  | BH    | 43  | ASN  |
| 30  | BH    | 73  | ASN  |
| 31  | BJ    | 67  | ASN  |
| 31  | BJ    | 80  | HIS  |
| 31  | BJ    | 128 | ASN  |
| 31  | BJ    | 131 | ASN  |
| 31  | BJ    | 135 | GLN  |
| 31  | BJ    | 136 | GLN  |
| 32  | BK    | 3   | GLN  |
| 32  | BK    | 5   | GLN  |
| 32  | BK    | 89  | ASN  |
| 33  | BL    | 54  | GLN  |
| 34  | BM    | 17  | ASN  |
| 34  | BM    | 45  | GLN  |
| 34  | BM    | 97  | GLN  |
| 35  | BN    | 9   | GLN  |
| 35  | BN    | 73  | ASN  |
| 35  | BN    | 81  | ASN  |
| 35  | BN    | 107 | ASN  |
| 36  | BO    | 19  | GLN  |
| 36  | BO    | 38  | GLN  |
| 36  | BO    | 67  | ASN  |
| 36  | BO    | 98  | GLN  |
| 36  | BO    | 104 | GLN  |
| 37  | BP    | 2   | ASN  |
| 37  | BP    | 11  | GLN  |
| 37  | BP    | 40  | GLN  |
| 37  | BP    | 114 | ASN  |
| 38  | BQ    | 36  | GLN  |
| 38  | BQ    | 43  | GLN  |
| 38  | BQ    | 51  | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | BQ    | 55  | GLN  |
| 38  | BQ    | 58  | GLN  |
| 38  | BQ    | 71  | ASN  |
| 38  | BQ    | 80  | ASN  |
| 39  | BR    | 11  | GLN  |
| 40  | BS    | 7   | HIS  |
| 40  | BS    | 9   | HIS  |
| 40  | BS    | 15  | GLN  |
| 40  | BS    | 57  | ASN  |
| 40  | BS    | 61  | ASN  |
| 41  | BT    | 28  | ASN  |
| 41  | BT    | 59  | ASN  |
| 41  | BT    | 91  | GLN  |
| 42  | BU    | 39  | ASN  |
| 42  | BU    | 65  | GLN  |
| 42  | BU    | 68  | ASN  |
| 43  | BW    | 49  | ASN  |
| 43  | BW    | 56  | HIS  |
| 44  | BX    | 38  | GLN  |
| 44  | BX    | 41  | HIS  |
| 44  | BX    | 45  | GLN  |
| 45  | BY    | 8   | GLN  |
| 45  | BY    | 19  | HIS  |
| 46  | BZ    | 65  | ASN  |
| 47  | B0    | 3   | GLN  |
| 47  | B0    | 4   | GLN  |
| 48  | B1    | 25  | ASN  |
| 48  | B1    | 45  | HIS  |
| 50  | B3    | 23  | HIS  |
| 51  | B4    | 13  | ASN  |
| 51  | B4    | 35  | GLN  |
| 51  | B4    | 37  | GLN  |
| 52  | BI    | 11  | GLN  |
| 52  | BI    | 29  | GLN  |
| 52  | BI    | 93  | ASN  |
| 2   | CC    | 2   | GLN  |
| 2   | CC    | 99  | GLN  |
| 2   | CC    | 189 | HIS  |
| 3   | CD    | 39  | GLN  |
| 3   | CD    | 53  | GLN  |
| 3   | CD    | 58  | GLN  |
| 3   | CD    | 99  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CD    | 115 | GLN  |
| 3   | CD    | 119 | HIS  |
| 3   | CD    | 130 | ASN  |
| 3   | CD    | 135 | GLN  |
| 3   | CD    | 151 | GLN  |
| 3   | CD    | 163 | GLN  |
| 3   | CD    | 195 | ASN  |
| 4   | CE    | 42  | ASN  |
| 4   | CE    | 72  | ASN  |
| 4   | CE    | 96  | GLN  |
| 4   | CE    | 131 | ASN  |
| 4   | CE    | 145 | ASN  |
| 5   | CF    | 17  | GLN  |
| 5   | CF    | 46  | GLN  |
| 5   | CF    | 63  | ASN  |
| 6   | CG    | 8   | GLN  |
| 6   | CG    | 27  | ASN  |
| 6   | CG    | 121 | ASN  |
| 7   | CH    | 37  | ASN  |
| 7   | CH    | 75  | GLN  |
| 7   | CH    | 117 | GLN  |
| 8   | CI    | 74  | GLN  |
| 8   | CI    | 80  | HIS  |
| 8   | CI    | 109 | GLN  |
| 8   | CI    | 125 | GLN  |
| 9   | CJ    | 58  | ASN  |
| 9   | CJ    | 99  | GLN  |
| 10  | CK    | 28  | ASN  |
| 10  | CK    | 37  | GLN  |
| 10  | CK    | 63  | GLN  |
| 10  | CK    | 108 | ASN  |
| 10  | CK    | 118 | ASN  |
| 11  | CL    | 28  | GLN  |
| 11  | CL    | 45  | ASN  |
| 11  | CL    | 58  | ASN  |
| 12  | CM    | 7   | ASN  |
| 13  | CN    | 34  | ASN  |
| 13  | CN    | 59  | GLN  |
| 13  | CN    | 61  | ASN  |
| 14  | CO    | 36  | ASN  |
| 15  | CP    | 26  | ASN  |
| 15  | CP    | 40  | ASN  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | CP    | 63  | GLN  |
| 16  | CQ    | 8   | GLN  |
| 16  | CQ    | 50  | ASN  |
| 17  | CR    | 51  | GLN  |
| 17  | CR    | 53  | GLN  |
| 18  | CS    | 42  | ASN  |
| 18  | CS    | 52  | ASN  |
| 18  | CS    | 55  | GLN  |
| 19  | CT    | 2   | ASN  |
| 19  | CT    | 12  | GLN  |
| 19  | CT    | 51  | ASN  |
| 19  | CT    | 69  | ASN  |
| 19  | CT    | 74  | HIS  |
| 19  | CT    | 83  | ASN  |
| 20  | CB    | 23  | ASN  |
| 20  | CB    | 38  | HIS  |
| 20  | CB    | 50  | ASN  |
| 20  | CB    | 119 | GLN  |
| 20  | CB    | 121 | GLN  |
| 20  | CB    | 145 | ASN  |
| 20  | CB    | 167 | HIS  |
| 20  | CB    | 202 | ASN  |
| 24  | DV    | 49  | ASN  |
| 24  | DV    | 51  | GLN  |
| 24  | DV    | 75  | GLN  |
| 24  | DV    | 78  | GLN  |
| 24  | DV    | 87  | GLN  |
| 25  | DC    | 20  | ASN  |
| 25  | DC    | 24  | HIS  |
| 25  | DC    | 43  | ASN  |
| 25  | DC    | 45  | ASN  |
| 25  | DC    | 57  | HIS  |
| 25  | DC    | 59  | GLN  |
| 25  | DC    | 116 | GLN  |
| 25  | DC    | 127 | ASN  |
| 25  | DC    | 141 | HIS  |
| 25  | DC    | 162 | GLN  |
| 25  | DC    | 196 | ASN  |
| 25  | DC    | 199 | HIS  |
| 25  | DC    | 225 | ASN  |
| 25  | DC    | 238 | ASN  |
| 26  | DD    | 36  | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | DD    | 94  | GLN  |
| 26  | DD    | 164 | GLN  |
| 26  | DD    | 173 | GLN  |
| 27  | DE    | 24  | ASN  |
| 27  | DE    | 30  | GLN  |
| 27  | DE    | 92  | HIS  |
| 27  | DE    | 94  | GLN  |
| 28  | DF    | 4   | HIS  |
| 28  | DF    | 36  | ASN  |
| 28  | DF    | 62  | GLN  |
| 28  | DF    | 80  | GLN  |
| 28  | DF    | 134 | GLN  |
| 29  | DG    | 29  | ASN  |
| 29  | DG    | 87  | GLN  |
| 29  | DG    | 100 | ASN  |
| 29  | DG    | 127 | GLN  |
| 29  | DG    | 138 | GLN  |
| 30  | DH    | 20  | ASN  |
| 30  | DH    | 28  | ASN  |
| 30  | DH    | 33  | GLN  |
| 30  | DH    | 133 | GLN  |
| 31  | DJ    | 86  | GLN  |
| 31  | DJ    | 135 | GLN  |
| 32  | DK    | 3   | GLN  |
| 33  | DL    | 38  | GLN  |
| 33  | DL    | 104 | GLN  |
| 34  | DM    | 3   | GLN  |
| 34  | DM    | 17  | ASN  |
| 34  | DM    | 22  | GLN  |
| 34  | DM    | 45  | GLN  |
| 34  | DM    | 97  | GLN  |
| 35  | DN    | 9   | GLN  |
| 35  | DN    | 11  | ASN  |
| 35  | DN    | 16  | HIS  |
| 35  | DN    | 18  | GLN  |
| 35  | DN    | 73  | ASN  |
| 35  | DN    | 107 | ASN  |
| 36  | DO    | 61  | GLN  |
| 36  | DO    | 67  | ASN  |
| 36  | DO    | 98  | GLN  |
| 36  | DO    | 104 | GLN  |
| 37  | DP    | 9   | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | DP    | 11  | GLN  |
| 37  | DP    | 55  | HIS  |
| 38  | DQ    | 13  | HIS  |
| 38  | DQ    | 43  | GLN  |
| 38  | DQ    | 51  | GLN  |
| 38  | DQ    | 58  | GLN  |
| 38  | DQ    | 71  | ASN  |
| 39  | DR    | 6   | GLN  |
| 39  | DR    | 43  | ASN  |
| 39  | DR    | 86  | GLN  |
| 40  | DS    | 15  | GLN  |
| 40  | DS    | 31  | GLN  |
| 40  | DS    | 40  | ASN  |
| 40  | DS    | 57  | ASN  |
| 41  | DT    | 48  | GLN  |
| 42  | DU    | 53  | GLN  |
| 42  | DU    | 65  | GLN  |
| 42  | DU    | 68  | ASN  |
| 43  | DW    | 2   | HIS  |
| 43  | DW    | 39  | GLN  |
| 43  | DW    | 45  | HIS  |
| 43  | DW    | 56  | HIS  |
| 44  | DX    | 31  | GLN  |
| 44  | DX    | 45  | GLN  |
| 44  | DX    | 58  | ASN  |
| 45  | DY    | 8   | GLN  |
| 45  | DY    | 48  | ASN  |
| 46  | DZ    | 65  | ASN  |
| 47  | D0    | 4   | GLN  |
| 48  | D1    | 44  | GLN  |
| 48  | D1    | 45  | HIS  |
| 49  | D2    | 29  | GLN  |
| 52  | DI    | 5   | GLN  |
| 52  | DI    | 33  | ASN  |
| 52  | DI    | 93  | ASN  |
| 52  | DI    | 106 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | AA    | 1529/1542 (99%) | 256 (16%)         | 24 (1%)         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | CA    | 1529/1542 (99%) | 232 (15%)         | 24 (1%)         |
| 22  | BA    | 116/120 (96%)   | 23 (19%)          | 0               |
| 22  | DA    | 116/120 (96%)   | 22 (18%)          | 0               |
| 23  | BB    | 2837/2904 (97%) | 424 (14%)         | 13 (0%)         |
| 23  | DB    | 2837/2904 (97%) | 438 (15%)         | 18 (0%)         |
| All | All   | 8964/9132 (98%) | 1395 (15%)        | 79 (0%)         |

All (1395) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 7   | A    |
| 1   | AA    | 9   | G    |
| 1   | AA    | 14  | U    |
| 1   | AA    | 32  | A    |
| 1   | AA    | 39  | G    |
| 1   | AA    | 47  | C    |
| 1   | AA    | 48  | C    |
| 1   | AA    | 51  | A    |
| 1   | AA    | 52  | C    |
| 1   | AA    | 55  | A    |
| 1   | AA    | 61  | G    |
| 1   | AA    | 66  | A    |
| 1   | AA    | 71  | A    |
| 1   | AA    | 72  | A    |
| 1   | AA    | 75  | G    |
| 1   | AA    | 78  | A    |
| 1   | AA    | 83  | C    |
| 1   | AA    | 85  | U    |
| 1   | AA    | 86  | G    |
| 1   | AA    | 87  | C    |
| 1   | AA    | 88  | U    |
| 1   | AA    | 89  | U    |
| 1   | AA    | 95  | C    |
| 1   | AA    | 108 | G    |
| 1   | AA    | 121 | U    |
| 1   | AA    | 122 | G    |
| 1   | AA    | 131 | A    |
| 1   | AA    | 151 | A    |
| 1   | AA    | 182 | A    |
| 1   | AA    | 197 | A    |
| 1   | AA    | 209 | U    |
| 1   | AA    | 210 | C    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 226 | G    |
| 1   | AA    | 239 | U    |
| 1   | AA    | 240 | G    |
| 1   | AA    | 243 | A    |
| 1   | AA    | 244 | U    |
| 1   | AA    | 245 | U    |
| 1   | AA    | 247 | G    |
| 1   | AA    | 250 | A    |
| 1   | AA    | 251 | G    |
| 1   | AA    | 257 | G    |
| 1   | AA    | 258 | G    |
| 1   | AA    | 266 | G    |
| 1   | AA    | 267 | C    |
| 1   | AA    | 280 | C    |
| 1   | AA    | 289 | G    |
| 1   | AA    | 316 | C    |
| 1   | AA    | 328 | C    |
| 1   | AA    | 329 | A    |
| 1   | AA    | 330 | C    |
| 1   | AA    | 332 | G    |
| 1   | AA    | 345 | C    |
| 1   | AA    | 351 | G    |
| 1   | AA    | 352 | C    |
| 1   | AA    | 354 | G    |
| 1   | AA    | 367 | U    |
| 1   | AA    | 372 | C    |
| 1   | AA    | 373 | A    |
| 1   | AA    | 381 | C    |
| 1   | AA    | 382 | A    |
| 1   | AA    | 397 | A    |
| 1   | AA    | 398 | U    |
| 1   | AA    | 406 | G    |
| 1   | AA    | 408 | A    |
| 1   | AA    | 409 | U    |
| 1   | AA    | 411 | A    |
| 1   | AA    | 412 | A    |
| 1   | AA    | 414 | A    |
| 1   | AA    | 415 | A    |
| 1   | AA    | 421 | U    |
| 1   | AA    | 422 | C    |
| 1   | AA    | 424 | G    |
| 1   | AA    | 429 | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 430 | A    |
| 1   | AA    | 435 | A    |
| 1   | AA    | 438 | U    |
| 1   | AA    | 461 | A    |
| 1   | AA    | 462 | G    |
| 1   | AA    | 463 | U    |
| 1   | AA    | 464 | U    |
| 1   | AA    | 465 | A    |
| 1   | AA    | 466 | A    |
| 1   | AA    | 467 | U    |
| 1   | AA    | 468 | A    |
| 1   | AA    | 469 | C    |
| 1   | AA    | 479 | U    |
| 1   | AA    | 481 | G    |
| 1   | AA    | 484 | G    |
| 1   | AA    | 485 | U    |
| 1   | AA    | 493 | A    |
| 1   | AA    | 518 | C    |
| 1   | AA    | 522 | C    |
| 1   | AA    | 527 | G    |
| 1   | AA    | 531 | U    |
| 1   | AA    | 532 | A    |
| 1   | AA    | 547 | A    |
| 1   | AA    | 559 | A    |
| 1   | AA    | 562 | U    |
| 1   | AA    | 564 | C    |
| 1   | AA    | 572 | A    |
| 1   | AA    | 573 | A    |
| 1   | AA    | 576 | C    |
| 1   | AA    | 577 | G    |
| 1   | AA    | 639 | G    |
| 1   | AA    | 650 | G    |
| 1   | AA    | 653 | U    |
| 1   | AA    | 665 | A    |
| 1   | AA    | 687 | A    |
| 1   | AA    | 700 | G    |
| 1   | AA    | 721 | G    |
| 1   | AA    | 724 | G    |
| 1   | AA    | 731 | G    |
| 1   | AA    | 733 | G    |
| 1   | AA    | 747 | A    |
| 1   | AA    | 748 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AA    | 755  | G    |
| 1   | AA    | 777  | A    |
| 1   | AA    | 781  | A    |
| 1   | AA    | 782  | A    |
| 1   | AA    | 793  | U    |
| 1   | AA    | 794  | A    |
| 1   | AA    | 812  | G    |
| 1   | AA    | 815  | A    |
| 1   | AA    | 817  | C    |
| 1   | AA    | 818  | G    |
| 1   | AA    | 819  | A    |
| 1   | AA    | 828  | U    |
| 1   | AA    | 829  | G    |
| 1   | AA    | 841  | C    |
| 1   | AA    | 842  | U    |
| 1   | AA    | 843  | U    |
| 1   | AA    | 844  | G    |
| 1   | AA    | 845  | A    |
| 1   | AA    | 846  | G    |
| 1   | AA    | 902  | G    |
| 1   | AA    | 914  | A    |
| 1   | AA    | 926  | G    |
| 1   | AA    | 927  | G    |
| 1   | AA    | 931  | C    |
| 1   | AA    | 934  | C    |
| 1   | AA    | 935  | A    |
| 1   | AA    | 960  | U    |
| 1   | AA    | 961  | U    |
| 1   | AA    | 966  | G    |
| 1   | AA    | 968  | A    |
| 1   | AA    | 969  | A    |
| 1   | AA    | 971  | G    |
| 1   | AA    | 974  | A    |
| 1   | AA    | 976  | G    |
| 1   | AA    | 977  | A    |
| 1   | AA    | 983  | A    |
| 1   | AA    | 991  | U    |
| 1   | AA    | 992  | U    |
| 1   | AA    | 993  | G    |
| 1   | AA    | 1002 | G    |
| 1   | AA    | 1004 | A    |
| 1   | AA    | 1009 | U    |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AA    | 1022 | A    |
| 1   | AA    | 1026 | G    |
| 1   | AA    | 1030 | U    |
| 1   | AA    | 1031 | C    |
| 1   | AA    | 1034 | G    |
| 1   | AA    | 1035 | A    |
| 1   | AA    | 1045 | C    |
| 1   | AA    | 1049 | U    |
| 1   | AA    | 1050 | G    |
| 1   | AA    | 1051 | C    |
| 1   | AA    | 1054 | C    |
| 1   | AA    | 1065 | U    |
| 1   | AA    | 1066 | C    |
| 1   | AA    | 1070 | U    |
| 1   | AA    | 1094 | G    |
| 1   | AA    | 1095 | U    |
| 1   | AA    | 1101 | A    |
| 1   | AA    | 1102 | A    |
| 1   | AA    | 1108 | G    |
| 1   | AA    | 1111 | A    |
| 1   | AA    | 1112 | C    |
| 1   | AA    | 1126 | U    |
| 1   | AA    | 1130 | A    |
| 1   | AA    | 1136 | C    |
| 1   | AA    | 1137 | C    |
| 1   | AA    | 1138 | G    |
| 1   | AA    | 1139 | G    |
| 1   | AA    | 1140 | C    |
| 1   | AA    | 1159 | U    |
| 1   | AA    | 1168 | U    |
| 1   | AA    | 1179 | A    |
| 1   | AA    | 1181 | G    |
| 1   | AA    | 1183 | U    |
| 1   | AA    | 1196 | A    |
| 1   | AA    | 1197 | A    |
| 1   | AA    | 1201 | A    |
| 1   | AA    | 1202 | U    |
| 1   | AA    | 1209 | C    |
| 1   | AA    | 1212 | U    |
| 1   | AA    | 1213 | A    |
| 1   | AA    | 1214 | C    |
| 1   | AA    | 1215 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AA    | 1225 | A    |
| 1   | AA    | 1226 | C    |
| 1   | AA    | 1227 | A    |
| 1   | AA    | 1228 | C    |
| 1   | AA    | 1240 | U    |
| 1   | AA    | 1241 | G    |
| 1   | AA    | 1253 | G    |
| 1   | AA    | 1256 | A    |
| 1   | AA    | 1258 | G    |
| 1   | AA    | 1261 | A    |
| 1   | AA    | 1278 | G    |
| 1   | AA    | 1279 | G    |
| 1   | AA    | 1280 | A    |
| 1   | AA    | 1281 | C    |
| 1   | AA    | 1285 | A    |
| 1   | AA    | 1286 | U    |
| 1   | AA    | 1298 | U    |
| 1   | AA    | 1300 | G    |
| 1   | AA    | 1301 | U    |
| 1   | AA    | 1305 | G    |
| 1   | AA    | 1316 | G    |
| 1   | AA    | 1317 | C    |
| 1   | AA    | 1320 | C    |
| 1   | AA    | 1322 | C    |
| 1   | AA    | 1323 | G    |
| 1   | AA    | 1336 | C    |
| 1   | AA    | 1346 | A    |
| 1   | AA    | 1347 | G    |
| 1   | AA    | 1353 | G    |
| 1   | AA    | 1362 | A    |
| 1   | AA    | 1363 | A    |
| 1   | AA    | 1364 | U    |
| 1   | AA    | 1378 | C    |
| 1   | AA    | 1379 | G    |
| 1   | AA    | 1380 | U    |
| 1   | AA    | 1381 | U    |
| 1   | AA    | 1398 | A    |
| 1   | AA    | 1404 | C    |
| 1   | AA    | 1409 | C    |
| 1   | AA    | 1419 | G    |
| 1   | AA    | 1432 | G    |
| 1   | AA    | 1446 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AA    | 1452 | C    |
| 1   | AA    | 1493 | A    |
| 1   | AA    | 1499 | A    |
| 1   | AA    | 1503 | A    |
| 1   | AA    | 1506 | U    |
| 1   | AA    | 1507 | A    |
| 1   | AA    | 1517 | G    |
| 1   | AA    | 1519 | A    |
| 1   | AA    | 1520 | C    |
| 1   | AA    | 1528 | U    |
| 1   | AA    | 1529 | G    |
| 1   | AA    | 1530 | G    |
| 1   | AA    | 1533 | C    |
| 1   | AA    | 1534 | A    |
| 22  | BA    | 11   | C    |
| 22  | BA    | 12   | C    |
| 22  | BA    | 13   | G    |
| 22  | BA    | 14   | U    |
| 22  | BA    | 15   | A    |
| 22  | BA    | 16   | G    |
| 22  | BA    | 25   | U    |
| 22  | BA    | 26   | C    |
| 22  | BA    | 28   | C    |
| 22  | BA    | 29   | A    |
| 22  | BA    | 30   | C    |
| 22  | BA    | 35   | C    |
| 22  | BA    | 42   | C    |
| 22  | BA    | 44   | G    |
| 22  | BA    | 45   | A    |
| 22  | BA    | 56   | G    |
| 22  | BA    | 66   | A    |
| 22  | BA    | 67   | G    |
| 22  | BA    | 84   | G    |
| 22  | BA    | 90   | C    |
| 22  | BA    | 99   | A    |
| 22  | BA    | 108  | A    |
| 22  | BA    | 109  | A    |
| 23  | BB    | 2    | G    |
| 23  | BB    | 4    | U    |
| 23  | BB    | 13   | A    |
| 23  | BB    | 14   | A    |
| 23  | BB    | 34   | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | BB    | 35  | G    |
| 23  | BB    | 46  | G    |
| 23  | BB    | 49  | A    |
| 23  | BB    | 63  | A    |
| 23  | BB    | 64  | A    |
| 23  | BB    | 71  | A    |
| 23  | BB    | 74  | A    |
| 23  | BB    | 75  | G    |
| 23  | BB    | 84  | A    |
| 23  | BB    | 85  | G    |
| 23  | BB    | 91  | A    |
| 23  | BB    | 92  | U    |
| 23  | BB    | 96  | C    |
| 23  | BB    | 100 | U    |
| 23  | BB    | 101 | A    |
| 23  | BB    | 102 | U    |
| 23  | BB    | 103 | A    |
| 23  | BB    | 104 | A    |
| 23  | BB    | 118 | A    |
| 23  | BB    | 119 | A    |
| 23  | BB    | 120 | U    |
| 23  | BB    | 125 | A    |
| 23  | BB    | 126 | A    |
| 23  | BB    | 140 | C    |
| 23  | BB    | 142 | A    |
| 23  | BB    | 144 | A    |
| 23  | BB    | 160 | A    |
| 23  | BB    | 162 | U    |
| 23  | BB    | 163 | C    |
| 23  | BB    | 181 | A    |
| 23  | BB    | 186 | G    |
| 23  | BB    | 196 | A    |
| 23  | BB    | 199 | A    |
| 23  | BB    | 209 | C    |
| 23  | BB    | 216 | A    |
| 23  | BB    | 221 | A    |
| 23  | BB    | 222 | A    |
| 23  | BB    | 230 | G    |
| 23  | BB    | 241 | A    |
| 23  | BB    | 248 | G    |
| 23  | BB    | 252 | G    |
| 23  | BB    | 255 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | BB    | 265 | A    |
| 23  | BB    | 266 | G    |
| 23  | BB    | 271 | G    |
| 23  | BB    | 277 | G    |
| 23  | BB    | 278 | A    |
| 23  | BB    | 279 | A    |
| 23  | BB    | 281 | C    |
| 23  | BB    | 311 | A    |
| 23  | BB    | 323 | C    |
| 23  | BB    | 329 | G    |
| 23  | BB    | 330 | A    |
| 23  | BB    | 353 | C    |
| 23  | BB    | 355 | U    |
| 23  | BB    | 362 | A    |
| 23  | BB    | 371 | A    |
| 23  | BB    | 372 | G    |
| 23  | BB    | 386 | G    |
| 23  | BB    | 387 | U    |
| 23  | BB    | 395 | U    |
| 23  | BB    | 396 | G    |
| 23  | BB    | 397 | U    |
| 23  | BB    | 411 | G    |
| 23  | BB    | 412 | A    |
| 23  | BB    | 423 | A    |
| 23  | BB    | 424 | G    |
| 23  | BB    | 435 | C    |
| 23  | BB    | 444 | C    |
| 23  | BB    | 455 | C    |
| 23  | BB    | 457 | A    |
| 23  | BB    | 479 | A    |
| 23  | BB    | 480 | A    |
| 23  | BB    | 481 | G    |
| 23  | BB    | 490 | C    |
| 23  | BB    | 491 | G    |
| 23  | BB    | 498 | G    |
| 23  | BB    | 504 | A    |
| 23  | BB    | 505 | A    |
| 23  | BB    | 508 | A    |
| 23  | BB    | 509 | C    |
| 23  | BB    | 512 | G    |
| 23  | BB    | 518 | G    |
| 23  | BB    | 527 | C    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | BB    | 531 | C    |
| 23  | BB    | 532 | A    |
| 23  | BB    | 533 | G    |
| 23  | BB    | 544 | C    |
| 23  | BB    | 545 | U    |
| 23  | BB    | 546 | U    |
| 23  | BB    | 547 | A    |
| 23  | BB    | 555 | G    |
| 23  | BB    | 563 | A    |
| 23  | BB    | 572 | A    |
| 23  | BB    | 573 | U    |
| 23  | BB    | 575 | A    |
| 23  | BB    | 588 | U    |
| 23  | BB    | 603 | A    |
| 23  | BB    | 613 | A    |
| 23  | BB    | 614 | A    |
| 23  | BB    | 615 | U    |
| 23  | BB    | 616 | A    |
| 23  | BB    | 627 | A    |
| 23  | BB    | 637 | A    |
| 23  | BB    | 645 | C    |
| 23  | BB    | 646 | U    |
| 23  | BB    | 654 | A    |
| 23  | BB    | 655 | A    |
| 23  | BB    | 671 | C    |
| 23  | BB    | 686 | U    |
| 23  | BB    | 717 | C    |
| 23  | BB    | 719 | C    |
| 23  | BB    | 722 | A    |
| 23  | BB    | 730 | A    |
| 23  | BB    | 747 | U    |
| 23  | BB    | 757 | G    |
| 23  | BB    | 765 | C    |
| 23  | BB    | 775 | G    |
| 23  | BB    | 782 | A    |
| 23  | BB    | 784 | G    |
| 23  | BB    | 785 | G    |
| 23  | BB    | 805 | G    |
| 23  | BB    | 812 | C    |
| 23  | BB    | 819 | A    |
| 23  | BB    | 827 | U    |
| 23  | BB    | 828 | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | BB    | 846  | U    |
| 23  | BB    | 847  | U    |
| 23  | BB    | 859  | G    |
| 23  | BB    | 872  | U    |
| 23  | BB    | 876  | C    |
| 23  | BB    | 877  | A    |
| 23  | BB    | 878  | A    |
| 23  | BB    | 899  | A    |
| 23  | BB    | 910  | A    |
| 23  | BB    | 912  | C    |
| 23  | BB    | 932  | U    |
| 23  | BB    | 933  | A    |
| 23  | BB    | 934  | U    |
| 23  | BB    | 941  | A    |
| 23  | BB    | 946  | C    |
| 23  | BB    | 955  | U    |
| 23  | BB    | 961  | C    |
| 23  | BB    | 973  | A    |
| 23  | BB    | 974  | G    |
| 23  | BB    | 983  | A    |
| 23  | BB    | 985  | C    |
| 23  | BB    | 991  | C    |
| 23  | BB    | 993  | G    |
| 23  | BB    | 995  | C    |
| 23  | BB    | 996  | A    |
| 23  | BB    | 1005 | C    |
| 23  | BB    | 1012 | U    |
| 23  | BB    | 1013 | C    |
| 23  | BB    | 1022 | G    |
| 23  | BB    | 1025 | G    |
| 23  | BB    | 1026 | G    |
| 23  | BB    | 1033 | U    |
| 23  | BB    | 1046 | A    |
| 23  | BB    | 1047 | G    |
| 23  | BB    | 1062 | G    |
| 23  | BB    | 1070 | A    |
| 23  | BB    | 1088 | A    |
| 23  | BB    | 1090 | A    |
| 23  | BB    | 1112 | G    |
| 23  | BB    | 1122 | G    |
| 23  | BB    | 1126 | A    |
| 23  | BB    | 1132 | U    |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | BB    | 1133 | A    |
| 23  | BB    | 1134 | A    |
| 23  | BB    | 1135 | C    |
| 23  | BB    | 1136 | G    |
| 23  | BB    | 1139 | G    |
| 23  | BB    | 1142 | A    |
| 23  | BB    | 1157 | G    |
| 23  | BB    | 1173 | U    |
| 23  | BB    | 1174 | U    |
| 23  | BB    | 1175 | A    |
| 23  | BB    | 1195 | G    |
| 23  | BB    | 1205 | A    |
| 23  | BB    | 1206 | G    |
| 23  | BB    | 1211 | C    |
| 23  | BB    | 1212 | G    |
| 23  | BB    | 1218 | G    |
| 23  | BB    | 1237 | A    |
| 23  | BB    | 1247 | A    |
| 23  | BB    | 1248 | G    |
| 23  | BB    | 1251 | C    |
| 23  | BB    | 1253 | A    |
| 23  | BB    | 1256 | G    |
| 23  | BB    | 1266 | G    |
| 23  | BB    | 1271 | G    |
| 23  | BB    | 1272 | A    |
| 23  | BB    | 1275 | A    |
| 23  | BB    | 1276 | A    |
| 23  | BB    | 1301 | A    |
| 23  | BB    | 1302 | A    |
| 23  | BB    | 1312 | U    |
| 23  | BB    | 1325 | U    |
| 23  | BB    | 1337 | G    |
| 23  | BB    | 1341 | G    |
| 23  | BB    | 1345 | C    |
| 23  | BB    | 1352 | U    |
| 23  | BB    | 1365 | A    |
| 23  | BB    | 1379 | U    |
| 23  | BB    | 1383 | A    |
| 23  | BB    | 1384 | A    |
| 23  | BB    | 1396 | U    |
| 23  | BB    | 1397 | U    |
| 23  | BB    | 1416 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | BB    | 1417 | C    |
| 23  | BB    | 1419 | A    |
| 23  | BB    | 1420 | A    |
| 23  | BB    | 1427 | A    |
| 23  | BB    | 1428 | C    |
| 23  | BB    | 1434 | A    |
| 23  | BB    | 1451 | C    |
| 23  | BB    | 1453 | A    |
| 23  | BB    | 1454 | C    |
| 23  | BB    | 1459 | G    |
| 23  | BB    | 1460 | U    |
| 23  | BB    | 1461 | C    |
| 23  | BB    | 1476 | U    |
| 23  | BB    | 1477 | A    |
| 23  | BB    | 1478 | G    |
| 23  | BB    | 1482 | G    |
| 23  | BB    | 1490 | A    |
| 23  | BB    | 1493 | C    |
| 23  | BB    | 1494 | A    |
| 23  | BB    | 1504 | A    |
| 23  | BB    | 1508 | A    |
| 23  | BB    | 1509 | A    |
| 23  | BB    | 1510 | G    |
| 23  | BB    | 1524 | G    |
| 23  | BB    | 1532 | A    |
| 23  | BB    | 1535 | A    |
| 23  | BB    | 1537 | G    |
| 23  | BB    | 1538 | G    |
| 23  | BB    | 1540 | G    |
| 23  | BB    | 1552 | A    |
| 23  | BB    | 1558 | C    |
| 23  | BB    | 1559 | U    |
| 23  | BB    | 1567 | G    |
| 23  | BB    | 1569 | A    |
| 23  | BB    | 1578 | U    |
| 23  | BB    | 1585 | C    |
| 23  | BB    | 1608 | A    |
| 23  | BB    | 1610 | A    |
| 23  | BB    | 1634 | A    |
| 23  | BB    | 1635 | A    |
| 23  | BB    | 1640 | A    |
| 23  | BB    | 1647 | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | BB    | 1648 | U    |
| 23  | BB    | 1649 | G    |
| 23  | BB    | 1674 | G    |
| 23  | BB    | 1700 | A    |
| 23  | BB    | 1701 | A    |
| 23  | BB    | 1706 | C    |
| 23  | BB    | 1707 | G    |
| 23  | BB    | 1713 | A    |
| 23  | BB    | 1715 | G    |
| 23  | BB    | 1716 | U    |
| 23  | BB    | 1722 | A    |
| 23  | BB    | 1723 | G    |
| 23  | BB    | 1729 | U    |
| 23  | BB    | 1730 | C    |
| 23  | BB    | 1731 | G    |
| 23  | BB    | 1733 | G    |
| 23  | BB    | 1738 | G    |
| 23  | BB    | 1758 | U    |
| 23  | BB    | 1764 | C    |
| 23  | BB    | 1773 | A    |
| 23  | BB    | 1781 | U    |
| 23  | BB    | 1800 | C    |
| 23  | BB    | 1816 | C    |
| 23  | BB    | 1829 | A    |
| 23  | BB    | 1833 | C    |
| 23  | BB    | 1870 | C    |
| 23  | BB    | 1873 | G    |
| 23  | BB    | 1876 | A    |
| 23  | BB    | 1884 | G    |
| 23  | BB    | 1906 | G    |
| 23  | BB    | 1914 | C    |
| 23  | BB    | 1927 | A    |
| 23  | BB    | 1929 | G    |
| 23  | BB    | 1930 | G    |
| 23  | BB    | 1937 | A    |
| 23  | BB    | 1938 | A    |
| 23  | BB    | 1939 | U    |
| 23  | BB    | 1940 | U    |
| 23  | BB    | 1955 | U    |
| 23  | BB    | 1966 | A    |
| 23  | BB    | 1967 | C    |
| 23  | BB    | 1970 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | BB    | 1971 | U    |
| 23  | BB    | 1972 | G    |
| 23  | BB    | 1991 | U    |
| 23  | BB    | 1993 | U    |
| 23  | BB    | 1997 | C    |
| 23  | BB    | 2022 | U    |
| 23  | BB    | 2023 | C    |
| 23  | BB    | 2031 | A    |
| 23  | BB    | 2033 | A    |
| 23  | BB    | 2043 | C    |
| 23  | BB    | 2055 | C    |
| 23  | BB    | 2056 | G    |
| 23  | BB    | 2060 | A    |
| 23  | BB    | 2061 | G    |
| 23  | BB    | 2062 | A    |
| 23  | BB    | 2069 | G    |
| 23  | BB    | 2072 | C    |
| 23  | BB    | 2102 | G    |
| 23  | BB    | 2104 | C    |
| 23  | BB    | 2105 | U    |
| 23  | BB    | 2137 | U    |
| 23  | BB    | 2140 | G    |
| 23  | BB    | 2144 | G    |
| 23  | BB    | 2145 | C    |
| 23  | BB    | 2147 | A    |
| 23  | BB    | 2149 | U    |
| 23  | BB    | 2154 | A    |
| 23  | BB    | 2181 | U    |
| 23  | BB    | 2183 | A    |
| 23  | BB    | 2187 | U    |
| 23  | BB    | 2192 | U    |
| 23  | BB    | 2198 | A    |
| 23  | BB    | 2204 | G    |
| 23  | BB    | 2212 | A    |
| 23  | BB    | 2225 | A    |
| 23  | BB    | 2238 | G    |
| 23  | BB    | 2239 | G    |
| 23  | BB    | 2259 | U    |
| 23  | BB    | 2266 | A    |
| 23  | BB    | 2273 | A    |
| 23  | BB    | 2276 | G    |
| 23  | BB    | 2278 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | BB    | 2283 | C    |
| 23  | BB    | 2286 | G    |
| 23  | BB    | 2287 | A    |
| 23  | BB    | 2297 | A    |
| 23  | BB    | 2304 | G    |
| 23  | BB    | 2305 | U    |
| 23  | BB    | 2307 | G    |
| 23  | BB    | 2318 | G    |
| 23  | BB    | 2319 | G    |
| 23  | BB    | 2320 | U    |
| 23  | BB    | 2321 | U    |
| 23  | BB    | 2322 | A    |
| 23  | BB    | 2325 | G    |
| 23  | BB    | 2333 | A    |
| 23  | BB    | 2334 | U    |
| 23  | BB    | 2336 | A    |
| 23  | BB    | 2337 | G    |
| 23  | BB    | 2347 | C    |
| 23  | BB    | 2383 | G    |
| 23  | BB    | 2385 | C    |
| 23  | BB    | 2402 | U    |
| 23  | BB    | 2403 | C    |
| 23  | BB    | 2406 | A    |
| 23  | BB    | 2423 | U    |
| 23  | BB    | 2426 | A    |
| 23  | BB    | 2429 | G    |
| 23  | BB    | 2430 | A    |
| 23  | BB    | 2434 | A    |
| 23  | BB    | 2441 | U    |
| 23  | BB    | 2448 | A    |
| 23  | BB    | 2472 | G    |
| 23  | BB    | 2476 | A    |
| 23  | BB    | 2491 | U    |
| 23  | BB    | 2492 | U    |
| 23  | BB    | 2502 | G    |
| 23  | BB    | 2505 | G    |
| 23  | BB    | 2506 | U    |
| 23  | BB    | 2518 | A    |
| 23  | BB    | 2529 | G    |
| 23  | BB    | 2535 | G    |
| 23  | BB    | 2554 | U    |
| 23  | BB    | 2566 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | BB    | 2567 | G    |
| 23  | BB    | 2573 | C    |
| 23  | BB    | 2585 | U    |
| 23  | BB    | 2586 | U    |
| 23  | BB    | 2597 | G    |
| 23  | BB    | 2602 | A    |
| 23  | BB    | 2609 | U    |
| 23  | BB    | 2613 | U    |
| 23  | BB    | 2621 | G    |
| 23  | BB    | 2629 | U    |
| 23  | BB    | 2654 | A    |
| 23  | BB    | 2682 | A    |
| 23  | BB    | 2689 | U    |
| 23  | BB    | 2690 | U    |
| 23  | BB    | 2714 | G    |
| 23  | BB    | 2725 | A    |
| 23  | BB    | 2726 | A    |
| 23  | BB    | 2744 | G    |
| 23  | BB    | 2748 | A    |
| 23  | BB    | 2751 | G    |
| 23  | BB    | 2752 | C    |
| 23  | BB    | 2757 | A    |
| 23  | BB    | 2765 | A    |
| 23  | BB    | 2778 | A    |
| 23  | BB    | 2791 | G    |
| 23  | BB    | 2796 | U    |
| 23  | BB    | 2797 | U    |
| 23  | BB    | 2800 | A    |
| 23  | BB    | 2801 | G    |
| 23  | BB    | 2808 | G    |
| 23  | BB    | 2820 | A    |
| 23  | BB    | 2821 | A    |
| 23  | BB    | 2836 | U    |
| 23  | BB    | 2850 | A    |
| 23  | BB    | 2866 | U    |
| 23  | BB    | 2867 | G    |
| 23  | BB    | 2872 | A    |
| 23  | BB    | 2873 | A    |
| 23  | BB    | 2883 | A    |
| 23  | BB    | 2894 | G    |
| 23  | BB    | 2903 | U    |
| 1   | CA    | 7    | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CA    | 9   | G    |
| 1   | CA    | 14  | U    |
| 1   | CA    | 32  | A    |
| 1   | CA    | 39  | G    |
| 1   | CA    | 47  | C    |
| 1   | CA    | 48  | C    |
| 1   | CA    | 51  | A    |
| 1   | CA    | 52  | C    |
| 1   | CA    | 55  | A    |
| 1   | CA    | 61  | G    |
| 1   | CA    | 71  | A    |
| 1   | CA    | 72  | A    |
| 1   | CA    | 83  | C    |
| 1   | CA    | 87  | C    |
| 1   | CA    | 92  | U    |
| 1   | CA    | 93  | U    |
| 1   | CA    | 94  | G    |
| 1   | CA    | 108 | G    |
| 1   | CA    | 121 | U    |
| 1   | CA    | 122 | G    |
| 1   | CA    | 131 | A    |
| 1   | CA    | 151 | A    |
| 1   | CA    | 182 | A    |
| 1   | CA    | 197 | A    |
| 1   | CA    | 209 | U    |
| 1   | CA    | 210 | C    |
| 1   | CA    | 226 | G    |
| 1   | CA    | 239 | U    |
| 1   | CA    | 240 | G    |
| 1   | CA    | 243 | A    |
| 1   | CA    | 244 | U    |
| 1   | CA    | 245 | U    |
| 1   | CA    | 247 | G    |
| 1   | CA    | 250 | A    |
| 1   | CA    | 251 | G    |
| 1   | CA    | 257 | G    |
| 1   | CA    | 258 | G    |
| 1   | CA    | 266 | G    |
| 1   | CA    | 267 | C    |
| 1   | CA    | 280 | C    |
| 1   | CA    | 289 | G    |
| 1   | CA    | 328 | C    |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CA    | 329 | A    |
| 1   | CA    | 330 | C    |
| 1   | CA    | 332 | G    |
| 1   | CA    | 345 | C    |
| 1   | CA    | 351 | G    |
| 1   | CA    | 352 | C    |
| 1   | CA    | 354 | G    |
| 1   | CA    | 367 | U    |
| 1   | CA    | 372 | C    |
| 1   | CA    | 373 | A    |
| 1   | CA    | 381 | C    |
| 1   | CA    | 382 | A    |
| 1   | CA    | 397 | A    |
| 1   | CA    | 398 | U    |
| 1   | CA    | 406 | G    |
| 1   | CA    | 408 | A    |
| 1   | CA    | 409 | U    |
| 1   | CA    | 411 | A    |
| 1   | CA    | 412 | A    |
| 1   | CA    | 414 | A    |
| 1   | CA    | 415 | A    |
| 1   | CA    | 421 | U    |
| 1   | CA    | 422 | C    |
| 1   | CA    | 424 | G    |
| 1   | CA    | 429 | U    |
| 1   | CA    | 430 | A    |
| 1   | CA    | 435 | A    |
| 1   | CA    | 438 | U    |
| 1   | CA    | 461 | A    |
| 1   | CA    | 462 | G    |
| 1   | CA    | 463 | U    |
| 1   | CA    | 464 | U    |
| 1   | CA    | 465 | A    |
| 1   | CA    | 466 | A    |
| 1   | CA    | 467 | U    |
| 1   | CA    | 468 | A    |
| 1   | CA    | 469 | C    |
| 1   | CA    | 479 | U    |
| 1   | CA    | 481 | G    |
| 1   | CA    | 484 | G    |
| 1   | CA    | 485 | U    |
| 1   | CA    | 493 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CA    | 518 | C    |
| 1   | CA    | 522 | C    |
| 1   | CA    | 527 | G    |
| 1   | CA    | 531 | U    |
| 1   | CA    | 532 | A    |
| 1   | CA    | 547 | A    |
| 1   | CA    | 559 | A    |
| 1   | CA    | 562 | U    |
| 1   | CA    | 564 | C    |
| 1   | CA    | 572 | A    |
| 1   | CA    | 573 | A    |
| 1   | CA    | 576 | C    |
| 1   | CA    | 577 | G    |
| 1   | CA    | 639 | G    |
| 1   | CA    | 650 | G    |
| 1   | CA    | 653 | U    |
| 1   | CA    | 665 | A    |
| 1   | CA    | 687 | A    |
| 1   | CA    | 700 | G    |
| 1   | CA    | 721 | G    |
| 1   | CA    | 724 | G    |
| 1   | CA    | 731 | G    |
| 1   | CA    | 733 | G    |
| 1   | CA    | 747 | A    |
| 1   | CA    | 748 | G    |
| 1   | CA    | 755 | G    |
| 1   | CA    | 777 | A    |
| 1   | CA    | 781 | A    |
| 1   | CA    | 782 | A    |
| 1   | CA    | 793 | U    |
| 1   | CA    | 794 | A    |
| 1   | CA    | 812 | G    |
| 1   | CA    | 815 | A    |
| 1   | CA    | 817 | C    |
| 1   | CA    | 818 | G    |
| 1   | CA    | 819 | A    |
| 1   | CA    | 828 | U    |
| 1   | CA    | 829 | G    |
| 1   | CA    | 841 | C    |
| 1   | CA    | 842 | U    |
| 1   | CA    | 843 | U    |
| 1   | CA    | 844 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | CA    | 845  | A    |
| 1   | CA    | 846  | G    |
| 1   | CA    | 907  | A    |
| 1   | CA    | 914  | A    |
| 1   | CA    | 926  | G    |
| 1   | CA    | 927  | G    |
| 1   | CA    | 934  | C    |
| 1   | CA    | 935  | A    |
| 1   | CA    | 945  | G    |
| 1   | CA    | 961  | U    |
| 1   | CA    | 969  | A    |
| 1   | CA    | 974  | A    |
| 1   | CA    | 976  | G    |
| 1   | CA    | 977  | A    |
| 1   | CA    | 991  | U    |
| 1   | CA    | 992  | U    |
| 1   | CA    | 993  | G    |
| 1   | CA    | 1004 | A    |
| 1   | CA    | 1009 | U    |
| 1   | CA    | 1010 | U    |
| 1   | CA    | 1020 | G    |
| 1   | CA    | 1022 | A    |
| 1   | CA    | 1023 | U    |
| 1   | CA    | 1025 | U    |
| 1   | CA    | 1031 | C    |
| 1   | CA    | 1033 | G    |
| 1   | CA    | 1034 | G    |
| 1   | CA    | 1036 | A    |
| 1   | CA    | 1044 | A    |
| 1   | CA    | 1050 | G    |
| 1   | CA    | 1053 | G    |
| 1   | CA    | 1054 | C    |
| 1   | CA    | 1065 | U    |
| 1   | CA    | 1066 | C    |
| 1   | CA    | 1091 | U    |
| 1   | CA    | 1094 | G    |
| 1   | CA    | 1095 | U    |
| 1   | CA    | 1101 | A    |
| 1   | CA    | 1118 | U    |
| 1   | CA    | 1129 | C    |
| 1   | CA    | 1130 | A    |
| 1   | CA    | 1135 | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | CA    | 1136 | C    |
| 1   | CA    | 1137 | C    |
| 1   | CA    | 1138 | G    |
| 1   | CA    | 1139 | G    |
| 1   | CA    | 1140 | C    |
| 1   | CA    | 1144 | G    |
| 1   | CA    | 1159 | U    |
| 1   | CA    | 1160 | G    |
| 1   | CA    | 1168 | U    |
| 1   | CA    | 1178 | G    |
| 1   | CA    | 1184 | G    |
| 1   | CA    | 1196 | A    |
| 1   | CA    | 1197 | A    |
| 1   | CA    | 1201 | A    |
| 1   | CA    | 1202 | U    |
| 1   | CA    | 1211 | U    |
| 1   | CA    | 1212 | U    |
| 1   | CA    | 1213 | A    |
| 1   | CA    | 1214 | C    |
| 1   | CA    | 1225 | A    |
| 1   | CA    | 1226 | C    |
| 1   | CA    | 1227 | A    |
| 1   | CA    | 1241 | G    |
| 1   | CA    | 1256 | A    |
| 1   | CA    | 1257 | A    |
| 1   | CA    | 1258 | G    |
| 1   | CA    | 1280 | A    |
| 1   | CA    | 1281 | C    |
| 1   | CA    | 1282 | C    |
| 1   | CA    | 1285 | A    |
| 1   | CA    | 1298 | U    |
| 1   | CA    | 1300 | G    |
| 1   | CA    | 1301 | U    |
| 1   | CA    | 1302 | C    |
| 1   | CA    | 1303 | C    |
| 1   | CA    | 1305 | G    |
| 1   | CA    | 1317 | C    |
| 1   | CA    | 1318 | A    |
| 1   | CA    | 1320 | C    |
| 1   | CA    | 1331 | G    |
| 1   | CA    | 1362 | A    |
| 1   | CA    | 1380 | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | CA    | 1397 | C    |
| 1   | CA    | 1398 | A    |
| 1   | CA    | 1400 | C    |
| 1   | CA    | 1401 | G    |
| 1   | CA    | 1419 | G    |
| 1   | CA    | 1426 | G    |
| 1   | CA    | 1432 | G    |
| 1   | CA    | 1446 | A    |
| 1   | CA    | 1452 | C    |
| 1   | CA    | 1493 | A    |
| 1   | CA    | 1497 | G    |
| 1   | CA    | 1503 | A    |
| 1   | CA    | 1505 | G    |
| 1   | CA    | 1506 | U    |
| 1   | CA    | 1507 | A    |
| 1   | CA    | 1517 | G    |
| 1   | CA    | 1520 | C    |
| 1   | CA    | 1529 | G    |
| 1   | CA    | 1530 | G    |
| 1   | CA    | 1533 | C    |
| 1   | CA    | 1534 | A    |
| 22  | DA    | 13   | G    |
| 22  | DA    | 15   | A    |
| 22  | DA    | 16   | G    |
| 22  | DA    | 18   | G    |
| 22  | DA    | 25   | U    |
| 22  | DA    | 26   | C    |
| 22  | DA    | 27   | C    |
| 22  | DA    | 28   | C    |
| 22  | DA    | 29   | A    |
| 22  | DA    | 42   | C    |
| 22  | DA    | 44   | G    |
| 22  | DA    | 52   | A    |
| 22  | DA    | 53   | A    |
| 22  | DA    | 56   | G    |
| 22  | DA    | 57   | A    |
| 22  | DA    | 66   | A    |
| 22  | DA    | 67   | G    |
| 22  | DA    | 89   | U    |
| 22  | DA    | 90   | C    |
| 22  | DA    | 91   | C    |
| 22  | DA    | 99   | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | DA    | 109 | A    |
| 23  | DB    | 12  | U    |
| 23  | DB    | 27  | G    |
| 23  | DB    | 35  | G    |
| 23  | DB    | 46  | G    |
| 23  | DB    | 49  | A    |
| 23  | DB    | 51  | G    |
| 23  | DB    | 52  | A    |
| 23  | DB    | 63  | A    |
| 23  | DB    | 64  | A    |
| 23  | DB    | 71  | A    |
| 23  | DB    | 74  | A    |
| 23  | DB    | 75  | G    |
| 23  | DB    | 91  | A    |
| 23  | DB    | 98  | G    |
| 23  | DB    | 99  | U    |
| 23  | DB    | 100 | U    |
| 23  | DB    | 101 | A    |
| 23  | DB    | 102 | U    |
| 23  | DB    | 103 | A    |
| 23  | DB    | 118 | A    |
| 23  | DB    | 119 | A    |
| 23  | DB    | 120 | U    |
| 23  | DB    | 124 | G    |
| 23  | DB    | 125 | A    |
| 23  | DB    | 126 | A    |
| 23  | DB    | 128 | C    |
| 23  | DB    | 139 | U    |
| 23  | DB    | 141 | G    |
| 23  | DB    | 144 | A    |
| 23  | DB    | 160 | A    |
| 23  | DB    | 162 | U    |
| 23  | DB    | 163 | C    |
| 23  | DB    | 180 | G    |
| 23  | DB    | 181 | A    |
| 23  | DB    | 196 | A    |
| 23  | DB    | 216 | A    |
| 23  | DB    | 221 | A    |
| 23  | DB    | 222 | A    |
| 23  | DB    | 223 | A    |
| 23  | DB    | 230 | G    |
| 23  | DB    | 233 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | DB    | 248 | G    |
| 23  | DB    | 250 | G    |
| 23  | DB    | 252 | G    |
| 23  | DB    | 255 | A    |
| 23  | DB    | 265 | A    |
| 23  | DB    | 266 | G    |
| 23  | DB    | 267 | C    |
| 23  | DB    | 271 | G    |
| 23  | DB    | 277 | G    |
| 23  | DB    | 278 | A    |
| 23  | DB    | 289 | G    |
| 23  | DB    | 299 | A    |
| 23  | DB    | 301 | G    |
| 23  | DB    | 302 | C    |
| 23  | DB    | 311 | A    |
| 23  | DB    | 312 | G    |
| 23  | DB    | 323 | C    |
| 23  | DB    | 329 | G    |
| 23  | DB    | 330 | A    |
| 23  | DB    | 333 | G    |
| 23  | DB    | 346 | A    |
| 23  | DB    | 353 | C    |
| 23  | DB    | 354 | A    |
| 23  | DB    | 361 | G    |
| 23  | DB    | 363 | G    |
| 23  | DB    | 365 | U    |
| 23  | DB    | 371 | A    |
| 23  | DB    | 372 | G    |
| 23  | DB    | 386 | G    |
| 23  | DB    | 387 | U    |
| 23  | DB    | 396 | G    |
| 23  | DB    | 403 | U    |
| 23  | DB    | 404 | A    |
| 23  | DB    | 405 | U    |
| 23  | DB    | 406 | G    |
| 23  | DB    | 411 | G    |
| 23  | DB    | 412 | A    |
| 23  | DB    | 424 | G    |
| 23  | DB    | 444 | C    |
| 23  | DB    | 448 | U    |
| 23  | DB    | 449 | A    |
| 23  | DB    | 455 | C    |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | DB    | 456 | C    |
| 23  | DB    | 457 | A    |
| 23  | DB    | 458 | G    |
| 23  | DB    | 475 | C    |
| 23  | DB    | 479 | A    |
| 23  | DB    | 480 | A    |
| 23  | DB    | 481 | G    |
| 23  | DB    | 491 | G    |
| 23  | DB    | 504 | A    |
| 23  | DB    | 505 | A    |
| 23  | DB    | 506 | G    |
| 23  | DB    | 508 | A    |
| 23  | DB    | 509 | C    |
| 23  | DB    | 512 | G    |
| 23  | DB    | 527 | C    |
| 23  | DB    | 530 | G    |
| 23  | DB    | 531 | C    |
| 23  | DB    | 532 | A    |
| 23  | DB    | 533 | G    |
| 23  | DB    | 544 | C    |
| 23  | DB    | 545 | U    |
| 23  | DB    | 546 | U    |
| 23  | DB    | 547 | A    |
| 23  | DB    | 548 | G    |
| 23  | DB    | 549 | G    |
| 23  | DB    | 550 | C    |
| 23  | DB    | 563 | A    |
| 23  | DB    | 572 | A    |
| 23  | DB    | 573 | U    |
| 23  | DB    | 575 | A    |
| 23  | DB    | 588 | U    |
| 23  | DB    | 603 | A    |
| 23  | DB    | 613 | A    |
| 23  | DB    | 614 | A    |
| 23  | DB    | 615 | U    |
| 23  | DB    | 616 | A    |
| 23  | DB    | 627 | A    |
| 23  | DB    | 637 | A    |
| 23  | DB    | 645 | C    |
| 23  | DB    | 646 | U    |
| 23  | DB    | 654 | A    |
| 23  | DB    | 655 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | DB    | 671 | C    |
| 23  | DB    | 686 | U    |
| 23  | DB    | 704 | G    |
| 23  | DB    | 718 | A    |
| 23  | DB    | 719 | C    |
| 23  | DB    | 727 | A    |
| 23  | DB    | 730 | A    |
| 23  | DB    | 747 | U    |
| 23  | DB    | 757 | G    |
| 23  | DB    | 765 | C    |
| 23  | DB    | 775 | G    |
| 23  | DB    | 782 | A    |
| 23  | DB    | 784 | G    |
| 23  | DB    | 785 | G    |
| 23  | DB    | 805 | G    |
| 23  | DB    | 812 | C    |
| 23  | DB    | 819 | A    |
| 23  | DB    | 827 | U    |
| 23  | DB    | 828 | U    |
| 23  | DB    | 844 | A    |
| 23  | DB    | 846 | U    |
| 23  | DB    | 847 | U    |
| 23  | DB    | 859 | G    |
| 23  | DB    | 869 | G    |
| 23  | DB    | 877 | A    |
| 23  | DB    | 899 | A    |
| 23  | DB    | 910 | A    |
| 23  | DB    | 912 | C    |
| 23  | DB    | 919 | U    |
| 23  | DB    | 931 | U    |
| 23  | DB    | 932 | U    |
| 23  | DB    | 933 | A    |
| 23  | DB    | 941 | A    |
| 23  | DB    | 946 | C    |
| 23  | DB    | 955 | U    |
| 23  | DB    | 961 | C    |
| 23  | DB    | 973 | A    |
| 23  | DB    | 974 | G    |
| 23  | DB    | 982 | C    |
| 23  | DB    | 983 | A    |
| 23  | DB    | 991 | C    |
| 23  | DB    | 995 | C    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | DB    | 1012 | U    |
| 23  | DB    | 1013 | C    |
| 23  | DB    | 1022 | G    |
| 23  | DB    | 1025 | G    |
| 23  | DB    | 1033 | U    |
| 23  | DB    | 1046 | A    |
| 23  | DB    | 1047 | G    |
| 23  | DB    | 1070 | A    |
| 23  | DB    | 1088 | A    |
| 23  | DB    | 1090 | A    |
| 23  | DB    | 1098 | A    |
| 23  | DB    | 1112 | G    |
| 23  | DB    | 1116 | G    |
| 23  | DB    | 1130 | U    |
| 23  | DB    | 1132 | U    |
| 23  | DB    | 1133 | A    |
| 23  | DB    | 1134 | A    |
| 23  | DB    | 1136 | G    |
| 23  | DB    | 1142 | A    |
| 23  | DB    | 1176 | U    |
| 23  | DB    | 1179 | G    |
| 23  | DB    | 1195 | G    |
| 23  | DB    | 1205 | A    |
| 23  | DB    | 1206 | G    |
| 23  | DB    | 1210 | G    |
| 23  | DB    | 1211 | C    |
| 23  | DB    | 1212 | G    |
| 23  | DB    | 1225 | G    |
| 23  | DB    | 1237 | A    |
| 23  | DB    | 1241 | A    |
| 23  | DB    | 1242 | U    |
| 23  | DB    | 1247 | A    |
| 23  | DB    | 1248 | G    |
| 23  | DB    | 1249 | U    |
| 23  | DB    | 1250 | G    |
| 23  | DB    | 1251 | C    |
| 23  | DB    | 1252 | G    |
| 23  | DB    | 1253 | A    |
| 23  | DB    | 1256 | G    |
| 23  | DB    | 1266 | G    |
| 23  | DB    | 1271 | G    |
| 23  | DB    | 1272 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | DB    | 1275 | A    |
| 23  | DB    | 1276 | A    |
| 23  | DB    | 1301 | A    |
| 23  | DB    | 1302 | A    |
| 23  | DB    | 1312 | U    |
| 23  | DB    | 1325 | U    |
| 23  | DB    | 1337 | G    |
| 23  | DB    | 1341 | G    |
| 23  | DB    | 1345 | C    |
| 23  | DB    | 1352 | U    |
| 23  | DB    | 1365 | A    |
| 23  | DB    | 1379 | U    |
| 23  | DB    | 1383 | A    |
| 23  | DB    | 1384 | A    |
| 23  | DB    | 1396 | U    |
| 23  | DB    | 1397 | U    |
| 23  | DB    | 1416 | G    |
| 23  | DB    | 1417 | C    |
| 23  | DB    | 1419 | A    |
| 23  | DB    | 1420 | A    |
| 23  | DB    | 1427 | A    |
| 23  | DB    | 1428 | C    |
| 23  | DB    | 1434 | A    |
| 23  | DB    | 1451 | C    |
| 23  | DB    | 1453 | A    |
| 23  | DB    | 1454 | C    |
| 23  | DB    | 1455 | G    |
| 23  | DB    | 1459 | G    |
| 23  | DB    | 1460 | U    |
| 23  | DB    | 1461 | C    |
| 23  | DB    | 1476 | U    |
| 23  | DB    | 1477 | A    |
| 23  | DB    | 1478 | G    |
| 23  | DB    | 1482 | G    |
| 23  | DB    | 1490 | A    |
| 23  | DB    | 1493 | C    |
| 23  | DB    | 1494 | A    |
| 23  | DB    | 1504 | A    |
| 23  | DB    | 1508 | A    |
| 23  | DB    | 1509 | A    |
| 23  | DB    | 1510 | G    |
| 23  | DB    | 1524 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | DB    | 1532 | A    |
| 23  | DB    | 1535 | A    |
| 23  | DB    | 1537 | G    |
| 23  | DB    | 1538 | G    |
| 23  | DB    | 1540 | G    |
| 23  | DB    | 1552 | A    |
| 23  | DB    | 1558 | C    |
| 23  | DB    | 1559 | U    |
| 23  | DB    | 1567 | G    |
| 23  | DB    | 1569 | A    |
| 23  | DB    | 1578 | U    |
| 23  | DB    | 1585 | C    |
| 23  | DB    | 1608 | A    |
| 23  | DB    | 1610 | A    |
| 23  | DB    | 1613 | G    |
| 23  | DB    | 1634 | A    |
| 23  | DB    | 1635 | A    |
| 23  | DB    | 1640 | A    |
| 23  | DB    | 1647 | U    |
| 23  | DB    | 1648 | U    |
| 23  | DB    | 1649 | G    |
| 23  | DB    | 1674 | G    |
| 23  | DB    | 1700 | A    |
| 23  | DB    | 1706 | C    |
| 23  | DB    | 1707 | G    |
| 23  | DB    | 1713 | A    |
| 23  | DB    | 1715 | G    |
| 23  | DB    | 1716 | U    |
| 23  | DB    | 1723 | G    |
| 23  | DB    | 1729 | U    |
| 23  | DB    | 1730 | C    |
| 23  | DB    | 1731 | G    |
| 23  | DB    | 1733 | G    |
| 23  | DB    | 1738 | G    |
| 23  | DB    | 1758 | U    |
| 23  | DB    | 1764 | C    |
| 23  | DB    | 1773 | A    |
| 23  | DB    | 1781 | U    |
| 23  | DB    | 1786 | A    |
| 23  | DB    | 1800 | C    |
| 23  | DB    | 1816 | C    |
| 23  | DB    | 1829 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | DB    | 1833 | C    |
| 23  | DB    | 1870 | C    |
| 23  | DB    | 1873 | G    |
| 23  | DB    | 1876 | A    |
| 23  | DB    | 1884 | G    |
| 23  | DB    | 1906 | G    |
| 23  | DB    | 1913 | A    |
| 23  | DB    | 1914 | C    |
| 23  | DB    | 1927 | A    |
| 23  | DB    | 1929 | G    |
| 23  | DB    | 1930 | G    |
| 23  | DB    | 1937 | A    |
| 23  | DB    | 1938 | A    |
| 23  | DB    | 1939 | U    |
| 23  | DB    | 1940 | U    |
| 23  | DB    | 1955 | U    |
| 23  | DB    | 1966 | A    |
| 23  | DB    | 1967 | C    |
| 23  | DB    | 1970 | A    |
| 23  | DB    | 1971 | U    |
| 23  | DB    | 1972 | G    |
| 23  | DB    | 1991 | U    |
| 23  | DB    | 1993 | U    |
| 23  | DB    | 1997 | C    |
| 23  | DB    | 2022 | U    |
| 23  | DB    | 2023 | C    |
| 23  | DB    | 2031 | A    |
| 23  | DB    | 2033 | A    |
| 23  | DB    | 2043 | C    |
| 23  | DB    | 2055 | C    |
| 23  | DB    | 2056 | G    |
| 23  | DB    | 2060 | A    |
| 23  | DB    | 2061 | G    |
| 23  | DB    | 2062 | A    |
| 23  | DB    | 2069 | G    |
| 23  | DB    | 2076 | U    |
| 23  | DB    | 2077 | A    |
| 23  | DB    | 2092 | U    |
| 23  | DB    | 2094 | A    |
| 23  | DB    | 2096 | C    |
| 23  | DB    | 2100 | G    |
| 23  | DB    | 2104 | C    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | DB    | 2106 | U    |
| 23  | DB    | 2107 | G    |
| 23  | DB    | 2109 | U    |
| 23  | DB    | 2134 | A    |
| 23  | DB    | 2135 | A    |
| 23  | DB    | 2138 | G    |
| 23  | DB    | 2143 | C    |
| 23  | DB    | 2145 | C    |
| 23  | DB    | 2147 | A    |
| 23  | DB    | 2156 | G    |
| 23  | DB    | 2157 | G    |
| 23  | DB    | 2181 | U    |
| 23  | DB    | 2183 | A    |
| 23  | DB    | 2190 | G    |
| 23  | DB    | 2199 | A    |
| 23  | DB    | 2204 | G    |
| 23  | DB    | 2210 | U    |
| 23  | DB    | 2212 | A    |
| 23  | DB    | 2225 | A    |
| 23  | DB    | 2239 | G    |
| 23  | DB    | 2253 | G    |
| 23  | DB    | 2268 | A    |
| 23  | DB    | 2283 | C    |
| 23  | DB    | 2287 | A    |
| 23  | DB    | 2288 | A    |
| 23  | DB    | 2297 | A    |
| 23  | DB    | 2305 | U    |
| 23  | DB    | 2307 | G    |
| 23  | DB    | 2308 | G    |
| 23  | DB    | 2309 | A    |
| 23  | DB    | 2310 | C    |
| 23  | DB    | 2319 | G    |
| 23  | DB    | 2321 | U    |
| 23  | DB    | 2322 | A    |
| 23  | DB    | 2325 | G    |
| 23  | DB    | 2333 | A    |
| 23  | DB    | 2334 | U    |
| 23  | DB    | 2336 | A    |
| 23  | DB    | 2337 | G    |
| 23  | DB    | 2347 | C    |
| 23  | DB    | 2383 | G    |
| 23  | DB    | 2385 | C    |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | DB    | 2402 | U    |
| 23  | DB    | 2403 | C    |
| 23  | DB    | 2406 | A    |
| 23  | DB    | 2423 | U    |
| 23  | DB    | 2426 | A    |
| 23  | DB    | 2429 | G    |
| 23  | DB    | 2430 | A    |
| 23  | DB    | 2434 | A    |
| 23  | DB    | 2441 | U    |
| 23  | DB    | 2448 | A    |
| 23  | DB    | 2472 | G    |
| 23  | DB    | 2476 | A    |
| 23  | DB    | 2491 | U    |
| 23  | DB    | 2492 | U    |
| 23  | DB    | 2502 | G    |
| 23  | DB    | 2505 | G    |
| 23  | DB    | 2506 | U    |
| 23  | DB    | 2518 | A    |
| 23  | DB    | 2529 | G    |
| 23  | DB    | 2535 | G    |
| 23  | DB    | 2554 | U    |
| 23  | DB    | 2566 | A    |
| 23  | DB    | 2567 | G    |
| 23  | DB    | 2573 | C    |
| 23  | DB    | 2585 | U    |
| 23  | DB    | 2586 | U    |
| 23  | DB    | 2597 | G    |
| 23  | DB    | 2602 | A    |
| 23  | DB    | 2609 | U    |
| 23  | DB    | 2610 | C    |
| 23  | DB    | 2613 | U    |
| 23  | DB    | 2621 | G    |
| 23  | DB    | 2629 | U    |
| 23  | DB    | 2654 | A    |
| 23  | DB    | 2682 | A    |
| 23  | DB    | 2689 | U    |
| 23  | DB    | 2690 | U    |
| 23  | DB    | 2714 | G    |
| 23  | DB    | 2725 | A    |
| 23  | DB    | 2726 | A    |
| 23  | DB    | 2744 | G    |
| 23  | DB    | 2757 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | DB    | 2765 | A    |
| 23  | DB    | 2778 | A    |
| 23  | DB    | 2791 | G    |
| 23  | DB    | 2796 | U    |
| 23  | DB    | 2797 | U    |
| 23  | DB    | 2800 | A    |
| 23  | DB    | 2801 | G    |
| 23  | DB    | 2808 | G    |
| 23  | DB    | 2820 | A    |
| 23  | DB    | 2821 | A    |
| 23  | DB    | 2836 | U    |
| 23  | DB    | 2850 | A    |
| 23  | DB    | 2866 | U    |
| 23  | DB    | 2867 | G    |
| 23  | DB    | 2872 | A    |
| 23  | DB    | 2873 | A    |
| 23  | DB    | 2883 | A    |
| 23  | DB    | 2894 | G    |
| 23  | DB    | 2903 | U    |

All (79) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AA    | 51   | A    |
| 1   | AA    | 60   | A    |
| 1   | AA    | 243  | A    |
| 1   | AA    | 279  | A    |
| 1   | AA    | 328  | C    |
| 1   | AA    | 366  | A    |
| 1   | AA    | 372  | C    |
| 1   | AA    | 428  | G    |
| 1   | AA    | 429  | U    |
| 1   | AA    | 484  | G    |
| 1   | AA    | 576  | C    |
| 1   | AA    | 913  | A    |
| 1   | AA    | 960  | U    |
| 1   | AA    | 975  | A    |
| 1   | AA    | 1049 | U    |
| 1   | AA    | 1065 | U    |
| 1   | AA    | 1101 | A    |
| 1   | AA    | 1181 | G    |
| 1   | AA    | 1201 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AA    | 1226 | C    |
| 1   | AA    | 1286 | U    |
| 1   | AA    | 1300 | G    |
| 1   | AA    | 1397 | C    |
| 1   | AA    | 1528 | U    |
| 23  | BB    | 63   | A    |
| 23  | BB    | 102  | U    |
| 23  | BB    | 162  | U    |
| 23  | BB    | 670  | A    |
| 23  | BB    | 1205 | A    |
| 23  | BB    | 1210 | G    |
| 23  | BB    | 1236 | G    |
| 23  | BB    | 1250 | G    |
| 23  | BB    | 1913 | A    |
| 23  | BB    | 2282 | G    |
| 23  | BB    | 2336 | A    |
| 23  | BB    | 2425 | A    |
| 23  | BB    | 2756 | U    |
| 1   | CA    | 51   | A    |
| 1   | CA    | 60   | A    |
| 1   | CA    | 243  | A    |
| 1   | CA    | 279  | A    |
| 1   | CA    | 328  | C    |
| 1   | CA    | 366  | A    |
| 1   | CA    | 372  | C    |
| 1   | CA    | 428  | G    |
| 1   | CA    | 429  | U    |
| 1   | CA    | 484  | G    |
| 1   | CA    | 960  | U    |
| 1   | CA    | 975  | A    |
| 1   | CA    | 1030 | U    |
| 1   | CA    | 1049 | U    |
| 1   | CA    | 1064 | G    |
| 1   | CA    | 1065 | U    |
| 1   | CA    | 1135 | U    |
| 1   | CA    | 1201 | A    |
| 1   | CA    | 1226 | C    |
| 1   | CA    | 1300 | G    |
| 1   | CA    | 1301 | U    |
| 1   | CA    | 1302 | C    |
| 1   | CA    | 1397 | C    |
| 1   | CA    | 1451 | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | DB    | 63   | A    |
| 23  | DB    | 125  | A    |
| 23  | DB    | 162  | U    |
| 23  | DB    | 199  | A    |
| 23  | DB    | 301  | G    |
| 23  | DB    | 544  | C    |
| 23  | DB    | 670  | A    |
| 23  | DB    | 982  | C    |
| 23  | DB    | 1205 | A    |
| 23  | DB    | 1210 | G    |
| 23  | DB    | 1211 | C    |
| 23  | DB    | 2076 | U    |
| 23  | DB    | 2198 | A    |
| 23  | DB    | 2282 | G    |
| 23  | DB    | 2286 | G    |
| 23  | DB    | 2336 | A    |
| 23  | DB    | 2425 | A    |
| 23  | DB    | 2756 | U    |

## 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 345 ligands modelled in this entry, 343 are monoatomic - leaving 2 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 53  | KSG  | AA    | 1601 | -    | 26,27,27     | 1.49 | 4 (15%)  | 31,40,40    | 1.06 | 3 (9%)   |
| 53  | KSG  | CA    | 1601 | -    | 26,27,27     | 1.59 | 3 (11%)  | 31,40,40    | 0.97 | 1 (3%)   |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 53  | KSG  | AA    | 1601 | -    | -       | 2/10/52/52 | 0/2/2/2 |
| 53  | KSG  | CA    | 1601 | -    | -       | 2/10/52/52 | 0/2/2/2 |

All (7) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 53  | AA    | 1601 | KSG  | C1-C12 | 2.66  | 1.57        | 1.52     |
| 53  | CA    | 1601 | KSG  | C1-C12 | 2.61  | 1.57        | 1.52     |
| 53  | CA    | 1601 | KSG  | O7-C1  | 2.56  | 1.48        | 1.41     |
| 53  | CA    | 1601 | KSG  | O1-C1  | 2.31  | 1.48        | 1.41     |
| 53  | AA    | 1601 | KSG  | O7-C1  | 2.20  | 1.47        | 1.41     |
| 53  | AA    | 1601 | KSG  | C4-C3  | 2.04  | 1.57        | 1.52     |
| 53  | AA    | 1601 | KSG  | C13-N2 | -2.04 | 1.31        | 1.35     |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 53  | AA    | 1601 | KSG  | C1-O1-C2 | -2.33 | 112.46      | 117.98   |
| 53  | AA    | 1601 | KSG  | C4-C3-C2 | 2.20  | 114.68      | 109.68   |
| 53  | AA    | 1601 | KSG  | C5-C4-C3 | 2.07  | 114.47      | 110.83   |
| 53  | CA    | 1601 | KSG  | C6-C7-C2 | 2.02  | 114.26      | 109.68   |

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms        |
|-----|-------|------|------|--------------|
| 53  | AA    | 1601 | KSG  | C12-C1-O1-C2 |
| 53  | CA    | 1601 | KSG  | C12-C1-O1-C2 |

*Continued on next page...*

*Continued from previous page...*

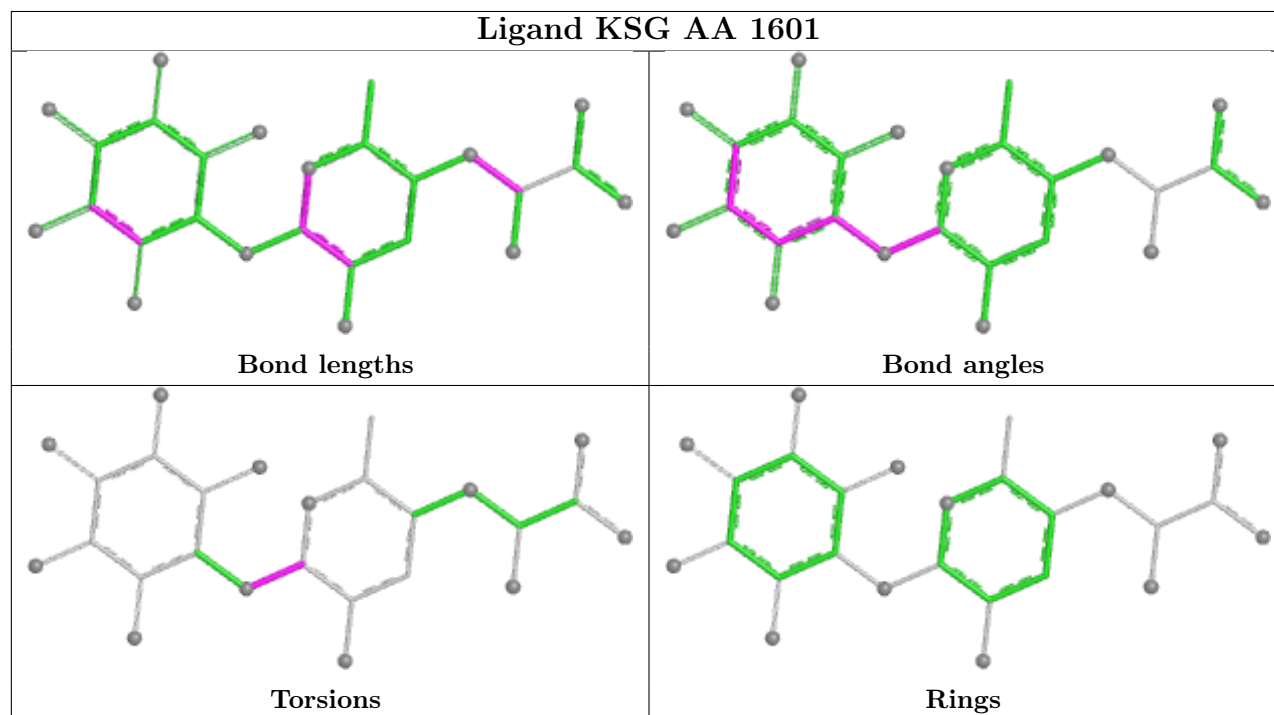
| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 53  | CA    | 1601 | KSG  | O7-C1-O1-C2 |
| 53  | AA    | 1601 | KSG  | O7-C1-O1-C2 |

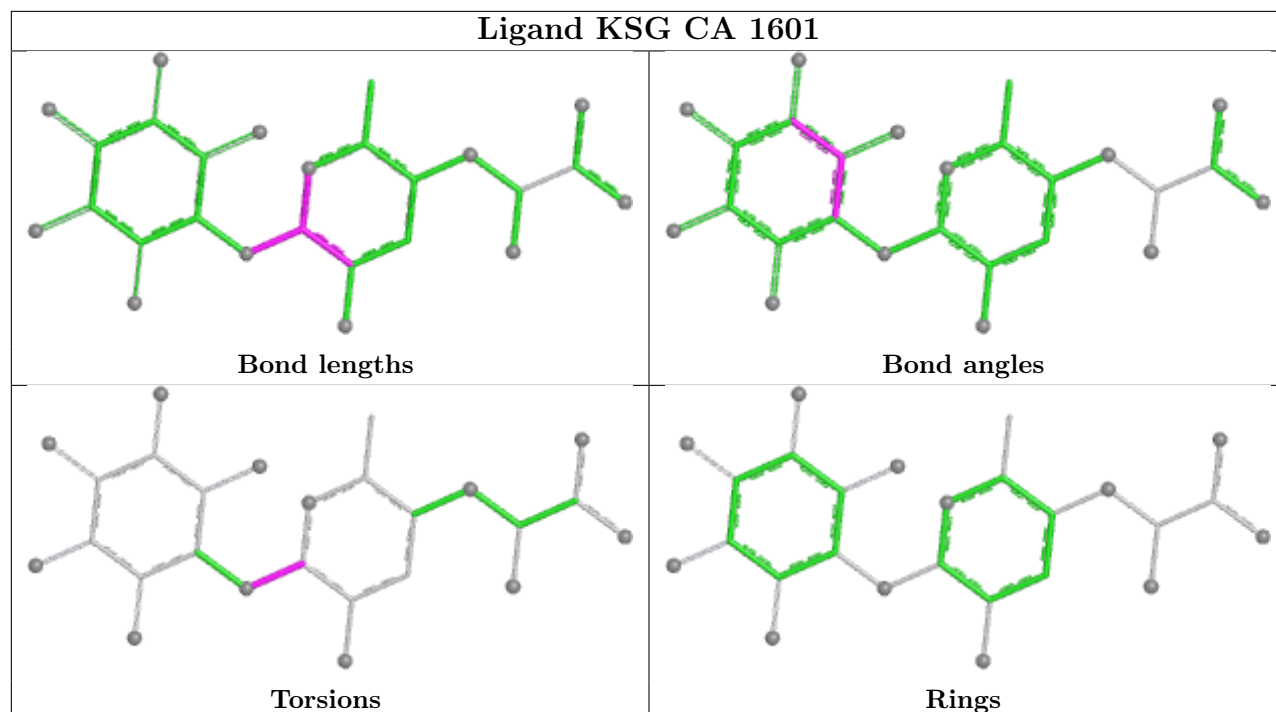
There are no ring outliers.

2 monomers are involved in 4 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 53  | AA    | 1601 | KSG  | 3       | 0            |
| 53  | CA    | 1601 | KSG  | 1       | 0            |

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





## 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   | AA    | 1530/1542 (99%) | 1.21   | 265 (17%) 4 4  | 15, 73, 149, 180      | 0     |
| 1   | CA    | 1530/1542 (99%) | 0.86   | 135 (8%) 15 11 | 7, 52, 134, 180       | 0     |
| 2   | AC    | 206/233 (88%)   | 1.22   | 50 (24%) 2 2   | 7, 68, 138, 180       | 0     |
| 2   | CC    | 206/233 (88%)   | 1.05   | 30 (14%) 6 5   | 6, 74, 126, 169       | 0     |
| 3   | AD    | 205/206 (99%)   | 1.75   | 78 (38%) 1 1   | 27, 79, 147, 180      | 0     |
| 3   | CD    | 205/206 (99%)   | 1.20   | 40 (19%) 3 3   | 5, 55, 113, 165       | 0     |
| 4   | AE    | 150/167 (89%)   | 1.22   | 34 (22%) 2 3   | 15, 62, 120, 162      | 0     |
| 4   | CE    | 150/167 (89%)   | 1.13   | 30 (20%) 3 3   | 6, 55, 112, 180       | 0     |
| 5   | AF    | 100/135 (74%)   | 1.22   | 19 (19%) 3 4   | 18, 72, 133, 166      | 0     |
| 5   | CF    | 100/135 (74%)   | 1.30   | 24 (24%) 2 2   | 12, 71, 132, 165      | 0     |
| 6   | AG    | 150/179 (83%)   | 1.35   | 36 (24%) 2 2   | 22, 89, 143, 180      | 0     |
| 6   | CG    | 152/179 (84%)   | 1.20   | 32 (21%) 2 3   | 19, 86, 147, 180      | 0     |
| 7   | AH    | 129/130 (99%)   | 1.53   | 38 (29%) 1 2   | 14, 70, 141, 176      | 0     |
| 7   | CH    | 129/130 (99%)   | 1.33   | 31 (24%) 2 2   | 5, 54, 114, 160       | 0     |
| 8   | AI    | 127/130 (97%)   | 1.46   | 37 (29%) 1 2   | 18, 90, 146, 180      | 0     |
| 8   | CI    | 127/130 (97%)   | 1.78   | 46 (36%) 1 1   | 23, 92, 156, 180      | 0     |
| 9   | AJ    | 98/103 (95%)    | 1.50   | 31 (31%) 1 1   | 20, 82, 157, 180      | 0     |
| 9   | CJ    | 98/103 (95%)    | 1.63   | 37 (37%) 1 1   | 34, 79, 135, 151      | 0     |
| 10  | AK    | 117/129 (90%)   | 1.42   | 28 (23%) 2 2   | 7, 55, 138, 160       | 0     |
| 10  | CK    | 117/129 (90%)   | 1.21   | 24 (20%) 2 3   | 11, 50, 105, 142      | 0     |
| 11  | AL    | 123/124 (99%)   | 1.89   | 48 (39%) 1 1   | 21, 61, 128, 178      | 0     |
| 11  | CL    | 123/124 (99%)   | 1.21   | 26 (21%) 2 3   | 5, 39, 119, 160       | 0     |
| 12  | AM    | 114/118 (96%)   | 1.37   | 27 (23%) 2 2   | 44, 106, 159, 173     | 0     |
| 12  | CM    | 113/118 (95%)   | 1.49   | 35 (30%) 1 2   | 26, 100, 157, 180     | 0     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2   |    |   | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|-----------|----|---|-----------------------|-------|
| 13  | AN    | 96/101 (95%)    | 1.89   | 43 (44%)  | 0  | 1 | 15, 84, 151, 180      | 0     |
| 13  | CN    | 96/101 (95%)    | 1.78   | 36 (37%)  | 1  | 1 | 21, 82, 139, 161      | 0     |
| 14  | AO    | 88/89 (98%)     | 1.56   | 31 (35%)  | 1  | 1 | 18, 70, 114, 180      | 0     |
| 14  | CO    | 88/89 (98%)     | 1.39   | 24 (27%)  | 1  | 2 | 14, 51, 112, 150      | 0     |
| 15  | AP    | 82/82 (100%)    | 1.70   | 26 (31%)  | 1  | 1 | 27, 89, 142, 180      | 0     |
| 15  | CP    | 80/82 (97%)     | 1.73   | 25 (31%)  | 1  | 1 | 5, 46, 145, 180       | 0     |
| 16  | AQ    | 80/84 (95%)     | 1.81   | 29 (36%)  | 1  | 1 | 37, 91, 140, 180      | 0     |
| 16  | CQ    | 81/84 (96%)     | 1.39   | 20 (24%)  | 2  | 2 | 12, 57, 119, 154      | 0     |
| 17  | AR    | 55/75 (73%)     | 1.77   | 18 (32%)  | 1  | 1 | 18, 69, 147, 164      | 0     |
| 17  | CR    | 55/75 (73%)     | 1.16   | 11 (20%)  | 3  | 3 | 13, 53, 126, 175      | 0     |
| 18  | AS    | 79/92 (85%)     | 1.74   | 27 (34%)  | 1  | 1 | 59, 112, 174, 180     | 0     |
| 18  | CS    | 80/92 (86%)     | 2.12   | 36 (45%)  | 0  | 1 | 48, 109, 172, 180     | 0     |
| 19  | AT    | 85/87 (97%)     | 2.06   | 34 (40%)  | 1  | 1 | 36, 94, 142, 170      | 0     |
| 19  | CT    | 85/87 (97%)     | 1.78   | 30 (35%)  | 1  | 1 | 17, 55, 118, 179      | 0     |
| 20  | AB    | 218/241 (90%)   | 1.25   | 51 (23%)  | 2  | 3 | 28, 92, 142, 180      | 0     |
| 20  | CB    | 218/241 (90%)   | 1.11   | 39 (17%)  | 3  | 4 | 26, 96, 157, 180      | 0     |
| 21  | AU    | 51/71 (71%)     | 2.33   | 27 (52%)  | 0  | 1 | 26, 94, 153, 174      | 0     |
| 21  | CU    | 51/71 (71%)     | 2.44   | 27 (52%)  | 0  | 1 | 29, 82, 163, 180      | 0     |
| 22  | BA    | 117/120 (97%)   | 1.12   | 13 (11%)  | 10 | 8 | 39, 67, 125, 171      | 0     |
| 22  | DA    | 117/120 (97%)   | 1.25   | 20 (17%)  | 4  | 4 | 34, 73, 116, 180      | 0     |
| 23  | BB    | 2841/2904 (97%) | 1.02   | 350 (12%) | 8  | 7 | 9, 53, 144, 180       | 0     |
| 23  | DB    | 2841/2904 (97%) | 0.93   | 278 (9%)  | 13 | 9 | 5, 45, 143, 180       | 0     |
| 24  | BV    | 94/94 (100%)    | 1.04   | 14 (14%)  | 5  | 5 | 26, 78, 134, 155      | 0     |
| 24  | DV    | 94/94 (100%)    | 1.56   | 26 (27%)  | 1  | 2 | 34, 83, 139, 162      | 0     |
| 25  | BC    | 267/273 (97%)   | 2.38   | 120 (44%) | 0  | 1 | 5, 53, 143, 180       | 0     |
| 25  | DC    | 267/273 (97%)   | 2.56   | 134 (50%) | 0  | 1 | 5, 52, 158, 180       | 0     |
| 26  | BD    | 209/209 (100%)  | 2.58   | 108 (51%) | 0  | 1 | 8, 82, 157, 180       | 0     |
| 26  | DD    | 209/209 (100%)  | 2.34   | 101 (48%) | 0  | 1 | 5, 57, 142, 180       | 0     |
| 27  | BE    | 201/201 (100%)  | 2.13   | 93 (46%)  | 0  | 1 | 5, 85, 162, 180       | 0     |
| 27  | DE    | 201/201 (100%)  | 2.45   | 107 (53%) | 0  | 1 | 6, 82, 170, 180       | 0     |
| 28  | BF    | 178/179 (99%)   | 1.51   | 48 (26%)  | 1  | 2 | 39, 105, 168, 180     | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2  |   |   | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|----------|---|---|-----------------------|-------|
| 28  | DF    | 178/179 (99%)  | 1.55   | 57 (32%) | 1 | 1 | 29, 96, 154, 180      | 0     |
| 29  | BG    | 176/177 (99%)  | 1.48   | 47 (26%) | 1 | 2 | 34, 100, 164, 180     | 0     |
| 29  | DG    | 176/177 (99%)  | 1.54   | 47 (26%) | 1 | 2 | 23, 88, 156, 180      | 0     |
| 30  | BH    | 149/149 (100%) | 1.61   | 41 (27%) | 1 | 2 | 22, 126, 180, 180     | 0     |
| 30  | DH    | 149/149 (100%) | 1.50   | 38 (25%) | 1 | 2 | 30, 106, 167, 180     | 0     |
| 31  | BJ    | 140/142 (98%)  | 2.61   | 78 (55%) | 0 | 1 | 11, 88, 153, 180      | 0     |
| 31  | DJ    | 140/142 (98%)  | 2.30   | 68 (48%) | 0 | 1 | 7, 66, 148, 176       | 0     |
| 32  | BK    | 121/123 (98%)  | 1.69   | 43 (35%) | 1 | 1 | 13, 60, 118, 152      | 0     |
| 32  | DK    | 121/123 (98%)  | 1.25   | 24 (19%) | 3 | 3 | 5, 36, 92, 134        | 0     |
| 33  | BL    | 144/144 (100%) | 3.52   | 88 (61%) | 0 | 1 | 15, 86, 167, 180      | 0     |
| 33  | DL    | 144/144 (100%) | 2.99   | 90 (62%) | 0 | 1 | 5, 81, 156, 180       | 0     |
| 34  | BM    | 136/136 (100%) | 2.52   | 73 (53%) | 0 | 1 | 13, 71, 175, 180      | 0     |
| 34  | DM    | 136/136 (100%) | 2.20   | 68 (50%) | 0 | 1 | 11, 70, 164, 180      | 0     |
| 35  | BN    | 127/127 (100%) | 2.81   | 66 (51%) | 0 | 1 | 17, 78, 168, 180      | 0     |
| 35  | DN    | 127/127 (100%) | 1.95   | 49 (38%) | 1 | 1 | 5, 48, 159, 180       | 0     |
| 36  | BO    | 117/117 (100%) | 2.66   | 63 (53%) | 0 | 1 | 26, 91, 167, 180      | 0     |
| 36  | DO    | 117/117 (100%) | 2.71   | 65 (55%) | 0 | 1 | 5, 91, 172, 180       | 0     |
| 37  | BP    | 114/115 (99%)  | 2.34   | 55 (48%) | 0 | 1 | 18, 98, 172, 180      | 0     |
| 37  | DP    | 114/115 (99%)  | 2.51   | 62 (54%) | 0 | 1 | 7, 65, 166, 180       | 0     |
| 38  | BQ    | 117/118 (99%)  | 2.18   | 52 (44%) | 0 | 1 | 13, 66, 146, 174      | 0     |
| 38  | DQ    | 117/118 (99%)  | 2.43   | 56 (47%) | 0 | 1 | 6, 57, 158, 180       | 0     |
| 39  | BR    | 103/103 (100%) | 2.59   | 61 (59%) | 0 | 1 | 24, 105, 167, 180     | 0     |
| 39  | DR    | 103/103 (100%) | 3.04   | 59 (57%) | 0 | 1 | 25, 92, 157, 180      | 0     |
| 40  | BS    | 110/110 (100%) | 2.06   | 37 (33%) | 1 | 1 | 9, 63, 133, 180       | 0     |
| 40  | DS    | 110/110 (100%) | 1.36   | 22 (20%) | 3 | 3 | 5, 46, 137, 180       | 0     |
| 41  | BT    | 99/100 (99%)   | 2.25   | 46 (46%) | 0 | 1 | 25, 81, 162, 180      | 0     |
| 41  | DT    | 99/100 (99%)   | 2.53   | 52 (52%) | 0 | 1 | 15, 86, 168, 180      | 0     |
| 42  | BU    | 102/104 (98%)  | 3.09   | 64 (62%) | 0 | 1 | 17, 91, 169, 180      | 0     |
| 42  | DU    | 102/104 (98%)  | 2.86   | 57 (55%) | 0 | 1 | 30, 110, 171, 180     | 0     |
| 43  | BW    | 84/85 (98%)    | 3.28   | 61 (72%) | 0 | 0 | 10, 86, 159, 180      | 0     |
| 43  | DW    | 84/85 (98%)    | 3.57   | 54 (64%) | 0 | 0 | 16, 86, 168, 180      | 0     |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2    |   |   | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|------------|---|---|-----------------------|-------|
| 44  | BX    | 63/63 (100%)      | 1.93   | 30 (47%)   | 0 | 1 | 20, 97, 160, 180      | 0     |
| 44  | DX    | 63/63 (100%)      | 2.56   | 31 (49%)   | 0 | 1 | 38, 110, 169, 180     | 0     |
| 45  | BY    | 58/59 (98%)       | 2.45   | 31 (53%)   | 0 | 1 | 13, 86, 157, 180      | 0     |
| 45  | DY    | 58/59 (98%)       | 2.23   | 24 (41%)   | 0 | 1 | 5, 79, 136, 150       | 0     |
| 46  | BZ    | 70/70 (100%)      | 2.73   | 36 (51%)   | 0 | 1 | 19, 66, 145, 180      | 0     |
| 46  | DZ    | 70/70 (100%)      | 3.23   | 47 (67%)   | 0 | 0 | 5, 68, 141, 180       | 0     |
| 47  | B0    | 56/57 (98%)       | 2.67   | 35 (62%)   | 0 | 1 | 26, 95, 180, 180      | 0     |
| 47  | D0    | 56/57 (98%)       | 2.46   | 30 (53%)   | 0 | 1 | 10, 70, 159, 177      | 0     |
| 48  | B1    | 54/55 (98%)       | 1.74   | 19 (35%)   | 1 | 1 | 24, 97, 160, 180      | 0     |
| 48  | D1    | 54/55 (98%)       | 1.88   | 23 (42%)   | 0 | 1 | 8, 82, 158, 180       | 0     |
| 49  | B2    | 46/46 (100%)      | 2.95   | 26 (56%)   | 0 | 1 | 6, 51, 154, 174       | 0     |
| 49  | D2    | 46/46 (100%)      | 3.07   | 33 (71%)   | 0 | 0 | 9, 55, 131, 150       | 0     |
| 50  | B3    | 64/65 (98%)       | 3.45   | 43 (67%)   | 0 | 0 | 19, 61, 155, 180      | 0     |
| 50  | D3    | 64/65 (98%)       | 3.25   | 41 (64%)   | 0 | 0 | 5, 61, 138, 178       | 0     |
| 51  | B4    | 38/38 (100%)      | 3.86   | 28 (73%)   | 0 | 0 | 30, 102, 170, 180     | 0     |
| 51  | D4    | 38/38 (100%)      | 4.23   | 30 (78%)   | 0 | 0 | 14, 111, 175, 180     | 0     |
| 52  | BI    | 141/142 (99%)     | 2.08   | 65 (46%)   | 0 | 1 | 52, 152, 180, 180     | 0     |
| 52  | DI    | 141/142 (99%)     | 1.79   | 53 (37%)   | 1 | 1 | 83, 160, 180, 180     | 0     |
| All | All   | 20439/21086 (96%) | 1.54   | 5495 (26%) | 1 | 2 | 5, 67, 155, 180       | 0     |

All (5495) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 23  | DB    | 2133 | G    | 16.0 |
| 43  | BW    | 45   | HIS  | 15.2 |
| 33  | DL    | 55   | MET  | 13.9 |
| 36  | DO    | 59   | ALA  | 13.5 |
| 40  | BS    | 93   | ALA  | 13.1 |
| 42  | BU    | 1    | ALA  | 13.1 |
| 33  | BL    | 34   | GLY  | 12.6 |
| 25  | DC    | 218  | THR  | 12.5 |
| 42  | BU    | 29   | SER  | 12.5 |
| 42  | DU    | 1    | ALA  | 12.4 |
| 39  | DR    | 53   | PHE  | 12.2 |
| 43  | DW    | 68   | PHE  | 12.0 |
| 36  | DO    | 58   | ILE  | 12.0 |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 25  | BC    | 241  | LYS  | 11.9 |
| 45  | BY    | 3    | THR  | 11.7 |
| 27  | DE    | 3    | LEU  | 11.7 |
| 33  | BL    | 77   | ILE  | 11.6 |
| 42  | DU    | 27   | VAL  | 11.5 |
| 23  | DB    | 2402 | U    | 11.3 |
| 25  | DC    | 85   | ASN  | 11.3 |
| 39  | DR    | 43   | ASN  | 11.2 |
| 26  | BD    | 135  | GLY  | 11.2 |
| 36  | DO    | 60   | GLU  | 11.0 |
| 25  | DC    | 209  | ALA  | 11.0 |
| 50  | B3    | 23   | HIS  | 10.9 |
| 25  | BC    | 268  | ARG  | 10.8 |
| 50  | B3    | 63   | TYR  | 10.7 |
| 51  | B4    | 23   | ILE  | 10.7 |
| 43  | DW    | 35   | ILE  | 10.7 |
| 33  | BL    | 27   | LEU  | 10.7 |
| 36  | BO    | 6    | ALA  | 10.6 |
| 26  | BD    | 134  | HIS  | 10.6 |
| 33  | BL    | 35   | HIS  | 10.5 |
| 39  | DR    | 44   | GLY  | 10.5 |
| 33  | BL    | 38   | GLN  | 10.5 |
| 35  | BN    | 20   | MET  | 10.4 |
| 35  | BN    | 67   | PHE  | 10.4 |
| 23  | BB    | 2308 | G    | 10.3 |
| 42  | BU    | 28   | LEU  | 10.3 |
| 42  | BU    | 89   | GLY  | 10.2 |
| 43  | BW    | 52   | CYS  | 10.2 |
| 33  | DL    | 52   | GLY  | 10.2 |
| 26  | BD    | 127  | PHE  | 10.2 |
| 51  | D4    | 23   | ILE  | 10.1 |
| 50  | B3    | 60   | CYS  | 10.1 |
| 50  | B3    | 57   | VAL  | 10.0 |
| 37  | DP    | 59   | THR  | 10.0 |
| 25  | BC    | 242  | HIS  | 9.9  |
| 49  | B2    | 14   | ARG  | 9.9  |
| 33  | BL    | 39   | LYS  | 9.9  |
| 39  | DR    | 78   | ARG  | 9.9  |
| 37  | DP    | 55   | HIS  | 9.8  |
| 8   | CI    | 129  | ARG  | 9.8  |
| 36  | DO    | 1    | MET  | 9.8  |
| 34  | BM    | 92   | TRP  | 9.8  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 29  | BG    | 1   | SER  | 9.8  |
| 43  | BW    | 68  | PHE  | 9.8  |
| 3   | AD    | 3   | TYR  | 9.7  |
| 25  | BC    | 247 | TRP  | 9.7  |
| 46  | BZ    | 22  | MET  | 9.7  |
| 35  | BN    | 6   | SER  | 9.7  |
| 27  | DE    | 171 | ASP  | 9.7  |
| 25  | BC    | 218 | THR  | 9.6  |
| 40  | BS    | 103 | ILE  | 9.5  |
| 26  | BD    | 133 | THR  | 9.5  |
| 43  | DW    | 73  | PRO  | 9.4  |
| 42  | BU    | 30  | SER  | 9.3  |
| 36  | BO    | 7   | ARG  | 9.3  |
| 40  | BS    | 92  | ARG  | 9.3  |
| 34  | BM    | 22  | GLN  | 9.2  |
| 46  | DZ    | 18  | CYS  | 9.2  |
| 51  | B4    | 38  | GLY  | 9.2  |
| 42  | BU    | 2   | ALA  | 9.2  |
| 16  | AQ    | 5   | ARG  | 9.2  |
| 36  | DO    | 3   | LYS  | 9.2  |
| 50  | B3    | 26  | ALA  | 9.2  |
| 25  | DC    | 257 | ARG  | 9.1  |
| 44  | DX    | 46  | VAL  | 9.1  |
| 42  | DU    | 32  | LYS  | 9.0  |
| 8   | CI    | 128 | LYS  | 9.0  |
| 38  | DQ    | 96  | ASP  | 9.0  |
| 29  | DG    | 172 | GLU  | 9.0  |
| 33  | DL    | 59  | ARG  | 9.0  |
| 33  | BL    | 73  | ILE  | 8.9  |
| 51  | D4    | 1   | MET  | 8.9  |
| 43  | DW    | 11  | ASN  | 8.9  |
| 49  | B2    | 15  | SER  | 8.8  |
| 33  | BL    | 54  | GLN  | 8.8  |
| 26  | BD    | 126 | ASN  | 8.8  |
| 36  | DO    | 57  | ALA  | 8.7  |
| 26  | DD    | 127 | PHE  | 8.7  |
| 51  | D4    | 31  | PRO  | 8.7  |
| 51  | B4    | 7   | VAL  | 8.6  |
| 25  | BC    | 251 | THR  | 8.6  |
| 33  | DL    | 45  | GLY  | 8.6  |
| 31  | DJ    | 88  | THR  | 8.6  |
| 34  | DM    | 18  | ARG  | 8.6  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 41  | BT    | 77   | ARG  | 8.6  |
| 41  | DT    | 74   | ILE  | 8.6  |
| 49  | B2    | 18   | PHE  | 8.6  |
| 25  | BC    | 239  | PHE  | 8.5  |
| 50  | D3    | 35   | LYS  | 8.5  |
| 26  | DD    | 49   | GLN  | 8.5  |
| 39  | BR    | 86   | GLN  | 8.5  |
| 39  | DR    | 87   | GLN  | 8.5  |
| 33  | BL    | 25   | SER  | 8.5  |
| 17  | AR    | 63   | TYR  | 8.5  |
| 22  | BA    | 88   | C    | 8.4  |
| 46  | BZ    | 33   | ASN  | 8.4  |
| 31  | BJ    | 82   | GLY  | 8.4  |
| 33  | BL    | 46   | VAL  | 8.3  |
| 22  | DA    | 88   | C    | 8.3  |
| 46  | BZ    | 63   | ARG  | 8.3  |
| 43  | DW    | 37   | VAL  | 8.3  |
| 33  | BL    | 12   | SER  | 8.3  |
| 35  | DN    | 57   | THR  | 8.3  |
| 33  | DL    | 53   | GLY  | 8.2  |
| 38  | BQ    | 90   | ASP  | 8.2  |
| 39  | BR    | 92   | TRP  | 8.2  |
| 50  | B3    | 64   | ALA  | 8.2  |
| 43  | DW    | 44   | PHE  | 8.2  |
| 25  | BC    | 20   | ASN  | 8.2  |
| 25  | BC    | 85   | ASN  | 8.2  |
| 30  | BH    | 12   | LEU  | 8.2  |
| 38  | DQ    | 54   | ARG  | 8.2  |
| 37  | DP    | 80   | VAL  | 8.1  |
| 42  | BU    | 61   | GLU  | 8.1  |
| 42  | DU    | 61   | GLU  | 8.1  |
| 25  | DC    | 246  | PRO  | 8.1  |
| 26  | BD    | 150  | GLN  | 8.1  |
| 50  | D3    | 36   | ALA  | 8.1  |
| 31  | DJ    | 102  | GLU  | 8.1  |
| 44  | DX    | 31   | GLN  | 8.1  |
| 25  | BC    | 256  | THR  | 8.1  |
| 31  | DJ    | 49   | ASP  | 8.0  |
| 23  | BB    | 2309 | A    | 8.0  |
| 42  | BU    | 32   | LYS  | 8.0  |
| 25  | DC    | 59   | GLN  | 8.0  |
| 31  | BJ    | 47   | HIS  | 8.0  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 33  | BL    | 52  | GLY  | 8.0  |
| 10  | CK    | 128 | VAL  | 7.9  |
| 33  | BL    | 8   | PRO  | 7.9  |
| 39  | DR    | 85  | LYS  | 7.9  |
| 51  | D4    | 33  | HIS  | 7.9  |
| 25  | DC    | 210 | ALA  | 7.9  |
| 50  | D3    | 33  | THR  | 7.9  |
| 7   | AH    | 1   | SER  | 7.9  |
| 50  | D3    | 53  | ASP  | 7.9  |
| 38  | BQ    | 35  | PHE  | 7.9  |
| 45  | DY    | 1   | ALA  | 7.9  |
| 49  | B2    | 13  | ASN  | 7.9  |
| 25  | DC    | 247 | TRP  | 7.9  |
| 31  | DJ    | 46  | PRO  | 7.8  |
| 33  | BL    | 40  | SER  | 7.8  |
| 36  | DO    | 61  | GLN  | 7.8  |
| 33  | BL    | 49  | GLY  | 7.8  |
| 36  | BO    | 97  | PHE  | 7.8  |
| 37  | BP    | 74  | GLN  | 7.8  |
| 7   | AH    | 2   | MET  | 7.8  |
| 51  | D4    | 7   | VAL  | 7.8  |
| 46  | BZ    | 27  | THR  | 7.8  |
| 33  | BL    | 56  | PRO  | 7.7  |
| 45  | BY    | 13  | ILE  | 7.7  |
| 50  | B3    | 61  | LEU  | 7.7  |
| 26  | BD    | 140 | HIS  | 7.7  |
| 33  | DL    | 42  | SER  | 7.7  |
| 1   | AA    | 121 | U    | 7.7  |
| 49  | B2    | 1   | MET  | 7.6  |
| 26  | DD    | 140 | HIS  | 7.6  |
| 35  | BN    | 102 | PHE  | 7.6  |
| 46  | BZ    | 4   | ASP  | 7.6  |
| 42  | DU    | 68  | ASN  | 7.6  |
| 35  | BN    | 64  | ARG  | 7.6  |
| 35  | BN    | 1   | MET  | 7.6  |
| 35  | BN    | 7   | GLY  | 7.6  |
| 5   | AF    | 52  | ASN  | 7.6  |
| 26  | DD    | 125 | TRP  | 7.5  |
| 41  | DT    | 77  | ARG  | 7.5  |
| 34  | DM    | 91  | TYR  | 7.5  |
| 50  | B3    | 44  | ARG  | 7.5  |
| 26  | BD    | 186 | LEU  | 7.5  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 51  | D4    | 38   | GLY  | 7.5  |
| 26  | BD    | 149  | ASN  | 7.5  |
| 11  | CL    | 85   | ARG  | 7.4  |
| 27  | DE    | 111  | GLU  | 7.4  |
| 31  | BJ    | 10   | THR  | 7.4  |
| 36  | BO    | 76   | LYS  | 7.4  |
| 42  | BU    | 14   | THR  | 7.4  |
| 41  | BT    | 79   | ASP  | 7.4  |
| 27  | BE    | 164  | LEU  | 7.4  |
| 35  | BN    | 2    | ARG  | 7.4  |
| 27  | DE    | 48   | THR  | 7.4  |
| 1   | AA    | 1362 | A    | 7.4  |
| 1   | CA    | 1362 | A    | 7.4  |
| 43  | DW    | 58   | LEU  | 7.3  |
| 10  | AK    | 128  | VAL  | 7.3  |
| 41  | DT    | 67   | VAL  | 7.3  |
| 8   | CI    | 65   | THR  | 7.3  |
| 33  | BL    | 37   | GLY  | 7.3  |
| 33  | DL    | 100  | ILE  | 7.3  |
| 27  | BE    | 158  | PHE  | 7.3  |
| 35  | BN    | 14   | SER  | 7.3  |
| 25  | DC    | 156  | SER  | 7.3  |
| 43  | BW    | 15   | SER  | 7.3  |
| 46  | BZ    | 10   | GLU  | 7.2  |
| 47  | B0    | 8    | THR  | 7.2  |
| 26  | BD    | 153  | GLY  | 7.2  |
| 33  | BL    | 62   | PRO  | 7.2  |
| 43  | DW    | 6    | GLY  | 7.2  |
| 25  | DC    | 268  | ARG  | 7.2  |
| 45  | DY    | 29   | ARG  | 7.2  |
| 18  | CS    | 2    | ARG  | 7.2  |
| 33  | BL    | 82   | LEU  | 7.2  |
| 39  | DR    | 77   | PHE  | 7.2  |
| 44  | DX    | 34   | SER  | 7.2  |
| 34  | DM    | 13   | HIS  | 7.2  |
| 37  | BP    | 24   | THR  | 7.1  |
| 33  | BL    | 57   | LEU  | 7.1  |
| 36  | BO    | 9    | ARG  | 7.1  |
| 25  | DC    | 224  | MET  | 7.1  |
| 26  | BD    | 9    | VAL  | 7.1  |
| 26  | DD    | 17   | GLU  | 7.1  |
| 43  | DW    | 39   | GLN  | 7.1  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 38  | BQ    | 111  | LYS  | 7.1  |
| 35  | DN    | 59   | SER  | 7.1  |
| 25  | DC    | 20   | ASN  | 7.1  |
| 27  | BE    | 129  | PRO  | 7.1  |
| 11  | AL    | 43   | LYS  | 7.1  |
| 1   | CA    | 121  | U    | 7.0  |
| 23  | DB    | 141  | G    | 7.0  |
| 51  | B4    | 4    | ARG  | 7.0  |
| 52  | DI    | 1    | ALA  | 7.0  |
| 51  | D4    | 37   | GLN  | 7.0  |
| 42  | DU    | 28   | LEU  | 7.0  |
| 25  | BC    | 258  | SER  | 7.0  |
| 43  | DW    | 3    | LYS  | 7.0  |
| 26  | DD    | 126  | ASN  | 7.0  |
| 51  | D4    | 25   | VAL  | 7.0  |
| 27  | DE    | 170  | ARG  | 7.0  |
| 38  | DQ    | 46   | TYR  | 7.0  |
| 26  | DD    | 33   | ARG  | 7.0  |
| 11  | AL    | 23   | LEU  | 6.9  |
| 33  | BL    | 19   | LEU  | 6.9  |
| 43  | BW    | 37   | VAL  | 6.9  |
| 25  | DC    | 57   | HIS  | 6.9  |
| 36  | DO    | 7    | ARG  | 6.9  |
| 6   | CG    | 105  | GLU  | 6.9  |
| 23  | DB    | 2134 | A    | 6.9  |
| 37  | DP    | 26   | GLU  | 6.9  |
| 50  | D3    | 62   | PRO  | 6.9  |
| 47  | B0    | 6    | LYS  | 6.9  |
| 43  | DW    | 52   | CYS  | 6.9  |
| 38  | DQ    | 51   | GLN  | 6.9  |
| 33  | DL    | 35   | HIS  | 6.9  |
| 25  | BC    | 21   | PRO  | 6.9  |
| 46  | DZ    | 22   | MET  | 6.9  |
| 50  | D3    | 28   | LEU  | 6.9  |
| 31  | BJ    | 48   | VAL  | 6.9  |
| 46  | DZ    | 20   | ASN  | 6.9  |
| 47  | B0    | 3    | GLN  | 6.9  |
| 25  | BC    | 43   | ASN  | 6.8  |
| 21  | CU    | 37   | TYR  | 6.8  |
| 38  | BQ    | 47   | ARG  | 6.8  |
| 29  | DG    | 59   | ASP  | 6.8  |
| 39  | DR    | 26   | ASP  | 6.8  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 38  | DQ    | 58   | GLN  | 6.8  |
| 13  | AN    | 60   | ARG  | 6.8  |
| 25  | BC    | 269  | ARG  | 6.8  |
| 50  | B3    | 29   | ARG  | 6.8  |
| 15  | CP    | 10   | GLY  | 6.8  |
| 51  | D4    | 3    | VAL  | 6.8  |
| 23  | DB    | 101  | A    | 6.7  |
| 51  | D4    | 5    | ALA  | 6.7  |
| 30  | DH    | 25   | TYR  | 6.7  |
| 31  | BJ    | 73   | VAL  | 6.7  |
| 31  | DJ    | 86   | GLN  | 6.7  |
| 34  | BM    | 83   | GLY  | 6.7  |
| 43  | DW    | 36   | ILE  | 6.7  |
| 25  | BC    | 57   | HIS  | 6.7  |
| 25  | BC    | 51   | ARG  | 6.7  |
| 50  | D3    | 32   | LEU  | 6.7  |
| 25  | DC    | 242  | HIS  | 6.6  |
| 36  | BO    | 58   | ILE  | 6.6  |
| 13  | AN    | 1    | ALA  | 6.6  |
| 23  | BB    | 2145 | C    | 6.6  |
| 44  | DX    | 36   | GLN  | 6.6  |
| 46  | DZ    | 41   | HIS  | 6.6  |
| 46  | BZ    | 32   | LEU  | 6.6  |
| 50  | D3    | 44   | ARG  | 6.6  |
| 22  | BA    | 52   | A    | 6.6  |
| 35  | BN    | 112  | TYR  | 6.6  |
| 25  | DC    | 3    | VAL  | 6.6  |
| 26  | DD    | 128  | ARG  | 6.6  |
| 27  | BE    | 104  | ALA  | 6.6  |
| 27  | BE    | 201  | ALA  | 6.6  |
| 38  | BQ    | 50   | ARG  | 6.6  |
| 38  | DQ    | 31   | TYR  | 6.6  |
| 39  | DR    | 83   | TYR  | 6.6  |
| 49  | B2    | 28   | ARG  | 6.6  |
| 33  | DL    | 38   | GLN  | 6.6  |
| 39  | DR    | 12   | HIS  | 6.6  |
| 25  | DC    | 244  | VAL  | 6.6  |
| 33  | DL    | 97   | ALA  | 6.6  |
| 37  | BP    | 23   | ASP  | 6.6  |
| 40  | BS    | 40   | ASN  | 6.5  |
| 16  | AQ    | 27   | PHE  | 6.5  |
| 31  | BJ    | 89   | PHE  | 6.5  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 39  | BR    | 11   | GLN  | 6.5  |
| 42  | DU    | 69   | VAL  | 6.5  |
| 19  | CT    | 35   | TYR  | 6.5  |
| 25  | BC    | 238  | ASN  | 6.5  |
| 43  | BW    | 36   | ILE  | 6.5  |
| 25  | DC    | 269  | ARG  | 6.5  |
| 25  | BC    | 224  | MET  | 6.5  |
| 46  | DZ    | 2    | LYS  | 6.5  |
| 51  | D4    | 20   | ASP  | 6.5  |
| 25  | BC    | 250  | GLN  | 6.5  |
| 43  | DW    | 45   | HIS  | 6.5  |
| 23  | DB    | 2833 | U    | 6.5  |
| 46  | DZ    | 27   | THR  | 6.5  |
| 25  | DC    | 261  | ARG  | 6.5  |
| 43  | DW    | 25   | PHE  | 6.5  |
| 37  | BP    | 96   | LEU  | 6.4  |
| 31  | BJ    | 44   | TYR  | 6.4  |
| 34  | DM    | 133  | LYS  | 6.4  |
| 22  | DA    | 28   | C    | 6.4  |
| 34  | BM    | 97   | GLN  | 6.4  |
| 35  | BN    | 71   | ARG  | 6.4  |
| 16  | AQ    | 36   | PHE  | 6.4  |
| 17  | AR    | 73   | HIS  | 6.4  |
| 31  | DJ    | 80   | HIS  | 6.4  |
| 26  | DD    | 90   | PHE  | 6.4  |
| 41  | DT    | 70   | HIS  | 6.4  |
| 47  | B0    | 9    | ARG  | 6.4  |
| 26  | DD    | 204  | LYS  | 6.4  |
| 51  | B4    | 28   | SER  | 6.4  |
| 21  | CU    | 34   | ARG  | 6.4  |
| 37  | BP    | 59   | THR  | 6.4  |
| 33  | BL    | 58   | TYR  | 6.4  |
| 36  | BO    | 52   | SER  | 6.4  |
| 23  | DB    | 140  | C    | 6.3  |
| 10  | CK    | 125  | LYS  | 6.3  |
| 25  | DC    | 259  | ASN  | 6.3  |
| 38  | DQ    | 91   | ARG  | 6.3  |
| 25  | BC    | 156  | SER  | 6.3  |
| 14  | CO    | 69   | LEU  | 6.3  |
| 24  | DV    | 14   | LYS  | 6.3  |
| 40  | BS    | 28   | LYS  | 6.3  |
| 27  | DE    | 108  | ILE  | 6.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 43  | BW    | 79  | ILE  | 6.3  |
| 42  | DU    | 41  | VAL  | 6.3  |
| 46  | BZ    | 9   | TYR  | 6.3  |
| 42  | BU    | 56  | GLY  | 6.3  |
| 25  | DC    | 19  | VAL  | 6.3  |
| 27  | DE    | 84  | THR  | 6.3  |
| 46  | DZ    | 9   | TYR  | 6.3  |
| 49  | D2    | 46  | LYS  | 6.3  |
| 23  | DB    | 139 | U    | 6.3  |
| 31  | BJ    | 4   | PHE  | 6.3  |
| 46  | DZ    | 58  | ASP  | 6.3  |
| 50  | D3    | 60  | CYS  | 6.3  |
| 45  | DY    | 11  | SER  | 6.3  |
| 50  | B3    | 30  | HIS  | 6.3  |
| 1   | CA    | 85  | U    | 6.3  |
| 25  | DC    | 136 | VAL  | 6.3  |
| 36  | BO    | 69  | ASP  | 6.2  |
| 27  | DE    | 86  | ALA  | 6.2  |
| 6   | AG    | 4   | ARG  | 6.2  |
| 33  | BL    | 33  | ARG  | 6.2  |
| 26  | BD    | 148 | GLN  | 6.2  |
| 42  | DU    | 60  | LYS  | 6.2  |
| 43  | BW    | 67  | LYS  | 6.2  |
| 17  | CR    | 19  | GLU  | 6.2  |
| 27  | DE    | 168 | ASP  | 6.2  |
| 52  | BI    | 1   | ALA  | 6.2  |
| 6   | AG    | 78  | ARG  | 6.2  |
| 3   | AD    | 6   | PRO  | 6.2  |
| 37  | DP    | 112 | ARG  | 6.2  |
| 27  | DE    | 169 | VAL  | 6.2  |
| 33  | BL    | 36  | LYS  | 6.2  |
| 39  | BR    | 91  | GLN  | 6.2  |
| 38  | BQ    | 49  | ARG  | 6.2  |
| 50  | D3    | 63  | TYR  | 6.2  |
| 41  | BT    | 65  | GLY  | 6.2  |
| 26  | BD    | 125 | TRP  | 6.2  |
| 45  | BY    | 24  | LEU  | 6.2  |
| 41  | DT    | 72  | GLN  | 6.2  |
| 11  | AL    | 110 | LYS  | 6.2  |
| 31  | DJ    | 89  | PHE  | 6.2  |
| 33  | BL    | 28  | GLY  | 6.2  |
| 33  | DL    | 107 | PHE  | 6.2  |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 50         | B3           | 42         | HIS         | 6.1         |
| 27         | BE           | 114        | ARG         | 6.1         |
| 49         | D2           | 19         | ARG         | 6.1         |
| 42         | DU           | 99         | SER         | 6.1         |
| 25         | DC           | 178        | GLY         | 6.1         |
| 25         | BC           | 209        | ALA         | 6.1         |
| 35         | DN           | 126        | ALA         | 6.1         |
| 26         | BD           | 14         | ILE         | 6.1         |
| 37         | BP           | 26         | GLU         | 6.1         |
| 37         | DP           | 97         | TYR         | 6.1         |
| 46         | DZ           | 64         | PHE         | 6.1         |
| 25         | BC           | 212        | TRP         | 6.1         |
| 11         | AL           | 25         | ALA         | 6.1         |
| 29         | DG           | 39         | ALA         | 6.1         |
| 46         | DZ           | 31         | ASP         | 6.1         |
| 51         | B4           | 15         | LYS         | 6.1         |
| 27         | BE           | 107        | SER         | 6.1         |
| 33         | DL           | 74         | THR         | 6.1         |
| 23         | BB           | 2148       | G           | 6.1         |
| 35         | BN           | 68         | ALA         | 6.1         |
| 23         | DB           | 508        | A           | 6.0         |
| 30         | BH           | 93         | SER         | 6.0         |
| 51         | D4           | 30         | GLU         | 6.0         |
| 25         | DC           | 256        | THR         | 6.0         |
| 39         | BR           | 12         | HIS         | 6.0         |
| 39         | DR           | 39         | LEU         | 6.0         |
| 41         | DT           | 37         | ASP         | 6.0         |
| 39         | BR           | 93         | PHE         | 6.0         |
| 42         | BU           | 59         | GLU         | 6.0         |
| 35         | DN           | 124        | ALA         | 6.0         |
| 1          | CA           | 461        | A           | 6.0         |
| 18         | CS           | 1          | PRO         | 6.0         |
| 27         | BE           | 59         | PRO         | 6.0         |
| 28         | DF           | 112        | ASP         | 6.0         |
| 41         | DT           | 68         | LYS         | 6.0         |
| 33         | DL           | 92         | LEU         | 6.0         |
| 47         | D0           | 55         | ALA         | 6.0         |
| 36         | DO           | 97         | PHE         | 6.0         |
| 21         | AU           | 35         | GLU         | 6.0         |
| 33         | DL           | 58         | TYR         | 6.0         |
| 37         | DP           | 61         | ARG         | 6.0         |
| 34         | BM           | 135        | VAL         | 5.9         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 26  | DD    | 79   | LEU  | 5.9  |
| 47  | B0    | 25   | THR  | 5.9  |
| 36  | BO    | 59   | ALA  | 5.9  |
| 36  | BO    | 56   | LYS  | 5.9  |
| 37  | BP    | 5    | LYS  | 5.9  |
| 27  | BE    | 60   | TRP  | 5.9  |
| 33  | DL    | 11   | GLY  | 5.9  |
| 26  | BD    | 132  | ALA  | 5.9  |
| 25  | BC    | 260  | LYS  | 5.9  |
| 33  | BL    | 50   | PHE  | 5.9  |
| 42  | BU    | 84   | PHE  | 5.9  |
| 23  | BB    | 1459 | G    | 5.9  |
| 33  | DL    | 57   | LEU  | 5.9  |
| 38  | DQ    | 4    | LYS  | 5.9  |
| 39  | DR    | 42   | ALA  | 5.9  |
| 40  | BS    | 34   | ASP  | 5.9  |
| 8   | CI    | 127  | SER  | 5.9  |
| 16  | AQ    | 4    | ILE  | 5.9  |
| 23  | DB    | 2147 | A    | 5.9  |
| 2   | AC    | 151  | GLU  | 5.9  |
| 33  | BL    | 99   | ASN  | 5.9  |
| 38  | BQ    | 91   | ARG  | 5.9  |
| 42  | BU    | 85   | ARG  | 5.9  |
| 33  | BL    | 32   | GLY  | 5.9  |
| 37  | BP    | 99   | LEU  | 5.9  |
| 27  | BE    | 144  | GLU  | 5.9  |
| 34  | DM    | 47   | GLU  | 5.9  |
| 23  | BB    | 645  | C    | 5.8  |
| 2   | CC    | 166  | TRP  | 5.8  |
| 26  | BD    | 147  | GLY  | 5.8  |
| 43  | DW    | 67   | LYS  | 5.8  |
| 38  | DQ    | 1    | ALA  | 5.8  |
| 34  | DM    | 89   | VAL  | 5.8  |
| 47  | D0    | 48   | TYR  | 5.8  |
| 25  | BC    | 29   | PHE  | 5.8  |
| 37  | DP    | 24   | THR  | 5.8  |
| 19  | CT    | 67   | HIS  | 5.8  |
| 1   | CA    | 1441 | A    | 5.8  |
| 44  | DX    | 28   | LEU  | 5.8  |
| 33  | BL    | 103  | ILE  | 5.8  |
| 6   | AG    | 76   | SER  | 5.8  |
| 37  | BP    | 97   | TYR  | 5.8  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 20  | AB    | 199 | ILE  | 5.8  |
| 31  | BJ    | 81  | ILE  | 5.8  |
| 25  | BC    | 60  | ALA  | 5.8  |
| 35  | BN    | 8   | ARG  | 5.8  |
| 26  | DD    | 136 | ASN  | 5.8  |
| 26  | DD    | 101 | PHE  | 5.8  |
| 21  | AU    | 37  | TYR  | 5.8  |
| 37  | BP    | 4   | ILE  | 5.8  |
| 28  | DF    | 171 | ALA  | 5.7  |
| 35  | BN    | 9   | GLN  | 5.7  |
| 46  | DZ    | 25  | ARG  | 5.7  |
| 46  | DZ    | 49  | ARG  | 5.7  |
| 13  | CN    | 72  | PHE  | 5.7  |
| 27  | DE    | 198 | GLU  | 5.7  |
| 26  | BD    | 129 | THR  | 5.7  |
| 13  | AN    | 55  | SER  | 5.7  |
| 36  | DO    | 8   | ILE  | 5.7  |
| 16  | CQ    | 6   | THR  | 5.7  |
| 27  | BE    | 67  | ARG  | 5.7  |
| 39  | DR    | 80  | ARG  | 5.7  |
| 25  | DC    | 239 | PHE  | 5.7  |
| 8   | AI    | 123 | ARG  | 5.7  |
| 26  | BD    | 152 | PRO  | 5.7  |
| 38  | DQ    | 32  | ARG  | 5.7  |
| 26  | DD    | 154 | LYS  | 5.7  |
| 31  | BJ    | 133 | ALA  | 5.7  |
| 47  | D0    | 44  | ALA  | 5.7  |
| 41  | DT    | 57  | VAL  | 5.7  |
| 26  | BD    | 123 | LYS  | 5.7  |
| 35  | BN    | 105 | GLY  | 5.7  |
| 40  | BS    | 83  | LYS  | 5.7  |
| 42  | BU    | 58  | VAL  | 5.7  |
| 6   | CG    | 108 | ARG  | 5.7  |
| 26  | DD    | 74  | GLU  | 5.7  |
| 31  | BJ    | 120 | ARG  | 5.7  |
| 42  | BU    | 88  | ASP  | 5.7  |
| 25  | DC    | 241 | LYS  | 5.6  |
| 31  | DJ    | 107 | GLY  | 5.6  |
| 33  | DL    | 28  | GLY  | 5.6  |
| 41  | DT    | 71  | GLY  | 5.6  |
| 31  | DJ    | 50  | THR  | 5.6  |
| 37  | BP    | 94  | ALA  | 5.6  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 51  | B4    | 17  | VAL  | 5.6  |
| 39  | BR    | 78  | ARG  | 5.6  |
| 38  | DQ    | 39  | ILE  | 5.6  |
| 43  | BW    | 11  | ASN  | 5.6  |
| 50  | D3    | 27  | ASN  | 5.6  |
| 33  | BL    | 70  | LYS  | 5.6  |
| 43  | BW    | 3   | LYS  | 5.6  |
| 49  | D2    | 37  | LYS  | 5.6  |
| 33  | DL    | 49  | GLY  | 5.6  |
| 39  | DR    | 64  | VAL  | 5.6  |
| 33  | BL    | 48  | ARG  | 5.6  |
| 51  | B4    | 24  | ARG  | 5.6  |
| 25  | DC    | 44  | ASN  | 5.6  |
| 36  | DO    | 64  | TYR  | 5.6  |
| 21  | AU    | 14  | ALA  | 5.6  |
| 36  | BO    | 5   | SER  | 5.6  |
| 8   | AI    | 67  | LYS  | 5.6  |
| 31  | BJ    | 46  | PRO  | 5.6  |
| 30  | BH    | 26  | ALA  | 5.6  |
| 25  | DC    | 199 | HIS  | 5.6  |
| 19  | AT    | 12  | GLN  | 5.6  |
| 41  | DT    | 4   | GLU  | 5.6  |
| 23  | DB    | 62  | U    | 5.6  |
| 45  | DY    | 12  | ALA  | 5.6  |
| 37  | DP    | 96  | LEU  | 5.6  |
| 21  | CU    | 33  | ARG  | 5.6  |
| 26  | DD    | 51  | THR  | 5.6  |
| 31  | BJ    | 7   | LYS  | 5.6  |
| 26  | BD    | 34  | VAL  | 5.5  |
| 34  | DM    | 57  | VAL  | 5.5  |
| 27  | DE    | 172 | ALA  | 5.5  |
| 40  | DS    | 95  | ARG  | 5.5  |
| 49  | B2    | 41  | ARG  | 5.5  |
| 31  | BJ    | 85  | LYS  | 5.5  |
| 25  | DC    | 9   | SER  | 5.5  |
| 33  | BL    | 7   | SER  | 5.5  |
| 47  | D0    | 33  | SER  | 5.5  |
| 23  | DB    | 645 | C    | 5.5  |
| 23  | DB    | 63  | A    | 5.5  |
| 27  | BE    | 200 | LEU  | 5.5  |
| 33  | DL    | 85  | VAL  | 5.5  |
| 34  | DM    | 109 | PRO  | 5.5  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 19  | AT    | 35  | TYR  | 5.5  |
| 43  | DW    | 79  | ILE  | 5.5  |
| 51  | B4    | 20  | ASP  | 5.5  |
| 29  | DG    | 169 | ARG  | 5.5  |
| 36  | BO    | 57  | ALA  | 5.5  |
| 44  | DX    | 1   | MET  | 5.5  |
| 17  | AR    | 36  | GLY  | 5.5  |
| 33  | BL    | 93  | ASN  | 5.5  |
| 27  | BE    | 49  | ARG  | 5.5  |
| 27  | BE    | 186 | VAL  | 5.5  |
| 38  | DQ    | 55  | GLN  | 5.5  |
| 42  | DU    | 92  | VAL  | 5.5  |
| 18  | AS    | 40  | PHE  | 5.5  |
| 20  | AB    | 212 | TYR  | 5.5  |
| 33  | DL    | 99  | ASN  | 5.5  |
| 49  | D2    | 43  | THR  | 5.5  |
| 25  | BC    | 257 | ARG  | 5.5  |
| 26  | DD    | 131 | ASP  | 5.5  |
| 26  | BD    | 116 | LYS  | 5.5  |
| 39  | DR    | 92  | TRP  | 5.5  |
| 51  | B4    | 1   | MET  | 5.5  |
| 41  | BT    | 38  | ALA  | 5.5  |
| 3   | AD    | 146 | GLU  | 5.5  |
| 25  | BC    | 41  | GLY  | 5.5  |
| 23  | DB    | 919 | U    | 5.5  |
| 25  | BC    | 127 | ASN  | 5.4  |
| 43  | DW    | 19  | ARG  | 5.4  |
| 24  | DV    | 76  | ASP  | 5.4  |
| 35  | DN    | 1   | MET  | 5.4  |
| 24  | DV    | 12  | GLN  | 5.4  |
| 32  | DK    | 71  | ARG  | 5.4  |
| 25  | BC    | 255 | LYS  | 5.4  |
| 46  | DZ    | 47  | LYS  | 5.4  |
| 30  | DH    | 122 | LEU  | 5.4  |
| 13  | AN    | 45  | LEU  | 5.4  |
| 18  | AS    | 13  | HIS  | 5.4  |
| 28  | DF    | 74  | ALA  | 5.4  |
| 34  | BM    | 64  | TRP  | 5.4  |
| 31  | BJ    | 119 | PHE  | 5.4  |
| 37  | BP    | 49  | ILE  | 5.4  |
| 17  | CR    | 63  | TYR  | 5.4  |
| 25  | BC    | 40  | GLY  | 5.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 33  | BL    | 64   | PHE  | 5.4  |
| 31  | DJ    | 84   | ILE  | 5.4  |
| 41  | DT    | 64   | LYS  | 5.4  |
| 34  | BM    | 56   | ALA  | 5.4  |
| 8   | CI    | 126  | PHE  | 5.4  |
| 25  | DC    | 41   | GLY  | 5.4  |
| 25  | DC    | 212  | TRP  | 5.4  |
| 26  | BD    | 146  | ILE  | 5.4  |
| 26  | BD    | 164  | GLN  | 5.4  |
| 25  | BC    | 199  | HIS  | 5.3  |
| 15  | CP    | 28   | ARG  | 5.3  |
| 26  | DD    | 151  | THR  | 5.3  |
| 27  | BE    | 48   | THR  | 5.3  |
| 39  | DR    | 5    | PHE  | 5.3  |
| 23  | DB    | 914  | G    | 5.3  |
| 41  | BT    | 32   | LEU  | 5.3  |
| 51  | B4    | 25   | VAL  | 5.3  |
| 38  | DQ    | 50   | ARG  | 5.3  |
| 10  | AK    | 125  | LYS  | 5.3  |
| 36  | BO    | 19   | GLN  | 5.3  |
| 27  | DE    | 153  | LEU  | 5.3  |
| 34  | BM    | 1    | MET  | 5.3  |
| 51  | D4    | 4    | ARG  | 5.3  |
| 23  | BB    | 1537 | G    | 5.3  |
| 31  | BJ    | 87   | ALA  | 5.3  |
| 31  | DJ    | 76   | HIS  | 5.3  |
| 33  | BL    | 71   | ALA  | 5.3  |
| 36  | DO    | 29   | HIS  | 5.3  |
| 51  | B4    | 29   | ALA  | 5.3  |
| 21  | AU    | 3    | ILE  | 5.3  |
| 25  | DC    | 7    | PRO  | 5.3  |
| 6   | AG    | 145  | GLU  | 5.3  |
| 11  | CL    | 24   | GLU  | 5.3  |
| 31  | DJ    | 91   | GLU  | 5.3  |
| 32  | BK    | 35   | VAL  | 5.3  |
| 18  | AS    | 36   | ARG  | 5.3  |
| 42  | BU    | 90   | LYS  | 5.3  |
| 19  | CT    | 62   | ALA  | 5.3  |
| 35  | BN    | 66   | ALA  | 5.3  |
| 35  | BN    | 3    | HIS  | 5.3  |
| 19  | AT    | 3    | ILE  | 5.3  |
| 44  | DX    | 35   | GLY  | 5.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 26  | DD    | 129  | THR  | 5.3  |
| 34  | BM    | 134  | THR  | 5.3  |
| 1   | CA    | 1031 | C    | 5.3  |
| 29  | DG    | 53   | PRO  | 5.3  |
| 45  | BY    | 17   | PRO  | 5.3  |
| 8   | CI    | 31   | GLN  | 5.3  |
| 23  | BB    | 1538 | G    | 5.3  |
| 26  | DD    | 59   | ARG  | 5.3  |
| 39  | BR    | 82   | HIS  | 5.3  |
| 33  | BL    | 22   | GLY  | 5.2  |
| 44  | DX    | 42   | LEU  | 5.2  |
| 13  | AN    | 66   | THR  | 5.2  |
| 35  | BN    | 69   | ARG  | 5.2  |
| 38  | DQ    | 12   | ARG  | 5.2  |
| 19  | CT    | 70   | LYS  | 5.2  |
| 29  | BG    | 58   | ALA  | 5.2  |
| 19  | AT    | 67   | HIS  | 5.2  |
| 40  | DS    | 108  | SER  | 5.2  |
| 42  | DU    | 29   | SER  | 5.2  |
| 21  | CU    | 44   | ARG  | 5.2  |
| 33  | DL    | 48   | ARG  | 5.2  |
| 30  | BH    | 33   | GLN  | 5.2  |
| 31  | DJ    | 7    | LYS  | 5.2  |
| 27  | DE    | 122  | GLU  | 5.2  |
| 36  | BO    | 1    | MET  | 5.2  |
| 4   | CE    | 126  | ALA  | 5.2  |
| 43  | DW    | 1    | ALA  | 5.2  |
| 35  | BN    | 51   | LEU  | 5.2  |
| 50  | B3    | 28   | LEU  | 5.2  |
| 47  | B0    | 34   | GLY  | 5.2  |
| 35  | DN    | 45   | ARG  | 5.2  |
| 3   | AD    | 120  | LYS  | 5.2  |
| 35  | BN    | 15   | SER  | 5.2  |
| 26  | BD    | 17   | GLU  | 5.2  |
| 6   | AG    | 116  | ALA  | 5.2  |
| 33  | BL    | 9    | ALA  | 5.2  |
| 36  | BO    | 92   | PHE  | 5.2  |
| 34  | BM    | 103  | TYR  | 5.2  |
| 25  | DC    | 208  | GLY  | 5.2  |
| 31  | BJ    | 80   | HIS  | 5.2  |
| 43  | DW    | 4    | LYS  | 5.2  |
| 23  | DB    | 34   | U    | 5.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 37  | DP    | 60   | VAL  | 5.2  |
| 36  | DO    | 24   | THR  | 5.2  |
| 3   | AD    | 143  | SER  | 5.2  |
| 11  | AL    | 123  | ALA  | 5.2  |
| 49  | D2    | 41   | ARG  | 5.2  |
| 33  | BL    | 24   | GLY  | 5.2  |
| 42  | DU    | 3    | LYS  | 5.2  |
| 25  | BC    | 267  | VAL  | 5.2  |
| 36  | BO    | 49   | VAL  | 5.2  |
| 26  | BD    | 130  | GLN  | 5.2  |
| 1   | AA    | 381  | C    | 5.1  |
| 38  | BQ    | 93   | ILE  | 5.1  |
| 34  | BM    | 55   | ARG  | 5.1  |
| 25  | DC    | 35   | LYS  | 5.1  |
| 19  | AT    | 69   | ASN  | 5.1  |
| 28  | BF    | 131  | VAL  | 5.1  |
| 34  | BM    | 98   | PRO  | 5.1  |
| 34  | BM    | 125  | PRO  | 5.1  |
| 23  | BB    | 1074 | G    | 5.1  |
| 18  | AS    | 11   | ASP  | 5.1  |
| 39  | DR    | 11   | GLN  | 5.1  |
| 41  | DT    | 80   | TRP  | 5.1  |
| 12  | CM    | 82   | LEU  | 5.1  |
| 18  | CS    | 34   | SER  | 5.1  |
| 19  | CT    | 63   | LYS  | 5.1  |
| 41  | BT    | 9    | LYS  | 5.1  |
| 49  | B2    | 35   | ARG  | 5.1  |
| 23  | BB    | 137  | U    | 5.1  |
| 43  | BW    | 53   | GLY  | 5.1  |
| 3   | CD    | 28   | ASP  | 5.1  |
| 21  | CU    | 41   | THR  | 5.1  |
| 31  | DJ    | 10   | THR  | 5.1  |
| 25  | DC    | 211  | ARG  | 5.1  |
| 33  | DL    | 101  | ILE  | 5.1  |
| 41  | DT    | 73   | ARG  | 5.1  |
| 46  | DZ    | 11   | GLU  | 5.1  |
| 43  | BW    | 51   | GLY  | 5.1  |
| 35  | BN    | 16   | HIS  | 5.1  |
| 50  | D3    | 7    | ARG  | 5.1  |
| 19  | CT    | 3    | ILE  | 5.1  |
| 31  | BJ    | 3    | THR  | 5.1  |
| 36  | DO    | 65   | THR  | 5.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 47  | D0    | 35   | GLU  | 5.1  |
| 49  | B2    | 6    | GLN  | 5.1  |
| 49  | B2    | 5    | PHE  | 5.1  |
| 10  | AK    | 49   | SER  | 5.1  |
| 43  | DW    | 29   | SER  | 5.1  |
| 11  | AL    | 97   | VAL  | 5.1  |
| 18  | CS    | 79   | TYR  | 5.1  |
| 25  | DC    | 103  | ILE  | 5.1  |
| 44  | DX    | 33   | ALA  | 5.1  |
| 34  | DM    | 132  | THR  | 5.1  |
| 35  | BN    | 127  | GLU  | 5.1  |
| 38  | BQ    | 36   | GLN  | 5.1  |
| 23  | DB    | 1205 | A    | 5.1  |
| 29  | DG    | 2    | ARG  | 5.1  |
| 39  | BR    | 79   | ARG  | 5.1  |
| 39  | DR    | 90   | ARG  | 5.1  |
| 47  | B0    | 38   | LEU  | 5.1  |
| 49  | D2    | 26   | ASN  | 5.1  |
| 31  | DJ    | 101  | ILE  | 5.0  |
| 43  | DW    | 83   | ALA  | 5.0  |
| 43  | DW    | 9    | THR  | 5.0  |
| 26  | DD    | 166  | GLY  | 5.0  |
| 30  | DH    | 21   | VAL  | 5.0  |
| 44  | BX    | 34   | SER  | 5.0  |
| 12  | CM    | 102  | LYS  | 5.0  |
| 28  | DF    | 68   | LYS  | 5.0  |
| 22  | DA    | 52   | A    | 5.0  |
| 39  | DR    | 82   | HIS  | 5.0  |
| 34  | BM    | 2    | LEU  | 5.0  |
| 49  | D2    | 7    | PRO  | 5.0  |
| 35  | BN    | 125  | ALA  | 5.0  |
| 33  | DL    | 50   | PHE  | 5.0  |
| 43  | BW    | 9    | THR  | 5.0  |
| 8   | AI    | 128  | LYS  | 5.0  |
| 21  | AU    | 44   | ARG  | 5.0  |
| 33  | DL    | 27   | LEU  | 5.0  |
| 52  | BI    | 127  | SER  | 5.0  |
| 42  | DU    | 2    | ALA  | 5.0  |
| 50  | D3    | 26   | ALA  | 5.0  |
| 25  | DC    | 225  | ASN  | 5.0  |
| 34  | BM    | 117  | PHE  | 5.0  |
| 1   | AA    | 1302 | C    | 5.0  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | CA    | 466  | A    | 5.0  |
| 23  | BB    | 1075 | C    | 5.0  |
| 23  | DB    | 1847 | A    | 5.0  |
| 38  | BQ    | 58   | GLN  | 5.0  |
| 39  | DR    | 62   | GLU  | 5.0  |
| 37  | BP    | 72   | VAL  | 5.0  |
| 49  | D2    | 28   | ARG  | 5.0  |
| 26  | BD    | 138  | LEU  | 5.0  |
| 25  | BC    | 37   | SER  | 5.0  |
| 15  | AP    | 81   | ALA  | 5.0  |
| 46  | DZ    | 44   | PHE  | 5.0  |
| 27  | DE    | 24   | ASN  | 5.0  |
| 23  | BB    | 2147 | A    | 5.0  |
| 37  | DP    | 68   | GLY  | 5.0  |
| 27  | DE    | 27   | LEU  | 5.0  |
| 43  | DW    | 20   | LEU  | 5.0  |
| 39  | BR    | 52   | PRO  | 5.0  |
| 42  | DU    | 44   | HIS  | 5.0  |
| 46  | BZ    | 5    | ILE  | 5.0  |
| 39  | BR    | 90   | ARG  | 5.0  |
| 31  | DJ    | 124  | VAL  | 5.0  |
| 34  | BM    | 26   | VAL  | 5.0  |
| 36  | BO    | 78   | VAL  | 5.0  |
| 21  | CU    | 42   | THR  | 5.0  |
| 25  | BC    | 59   | GLN  | 5.0  |
| 26  | BD    | 64   | GLU  | 5.0  |
| 31  | BJ    | 98   | GLU  | 5.0  |
| 34  | BM    | 19   | GLY  | 5.0  |
| 33  | DL    | 56   | PRO  | 4.9  |
| 1   | CA    | 977  | A    | 4.9  |
| 30  | DH    | 23   | ALA  | 4.9  |
| 42  | DU    | 91   | LYS  | 4.9  |
| 27  | BE    | 188  | MET  | 4.9  |
| 23  | BB    | 2402 | U    | 4.9  |
| 34  | BM    | 3    | GLN  | 4.9  |
| 36  | BO    | 43   | ASN  | 4.9  |
| 46  | DZ    | 48   | GLN  | 4.9  |
| 42  | BU    | 38   | ILE  | 4.9  |
| 39  | BR    | 77   | PHE  | 4.9  |
| 43  | DW    | 63   | ASP  | 4.9  |
| 10  | AK    | 91   | GLY  | 4.9  |
| 25  | DC    | 8    | THR  | 4.9  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 45  | DY    | 32   | GLY  | 4.9  |
| 46  | BZ    | 13   | THR  | 4.9  |
| 30  | DH    | 72   | ILE  | 4.9  |
| 33  | DL    | 73   | ILE  | 4.9  |
| 33  | DL    | 62   | PRO  | 4.9  |
| 41  | BT    | 64   | LYS  | 4.9  |
| 43  | BW    | 4    | LYS  | 4.9  |
| 8   | CI    | 63   | TYR  | 4.9  |
| 29  | BG    | 93   | TYR  | 4.9  |
| 38  | DQ    | 87   | VAL  | 4.9  |
| 26  | DD    | 145  | SER  | 4.9  |
| 26  | BD    | 198  | GLY  | 4.9  |
| 27  | DE    | 42   | GLY  | 4.9  |
| 33  | DL    | 67   | THR  | 4.9  |
| 52  | DI    | 9    | LYS  | 4.9  |
| 1   | CA    | 1032 | G    | 4.9  |
| 29  | DG    | 51   | PHE  | 4.9  |
| 50  | B3    | 13   | PHE  | 4.9  |
| 27  | DE    | 92   | HIS  | 4.9  |
| 7   | AH    | 33   | VAL  | 4.9  |
| 2   | AC    | 160  | GLU  | 4.9  |
| 27  | DE    | 155  | GLU  | 4.9  |
| 41  | BT    | 80   | TRP  | 4.9  |
| 26  | BD    | 25   | THR  | 4.9  |
| 33  | DL    | 4    | ASN  | 4.9  |
| 25  | BC    | 7    | PRO  | 4.9  |
| 50  | D3    | 64   | ALA  | 4.9  |
| 46  | DZ    | 43   | PHE  | 4.9  |
| 46  | DZ    | 6    | HIS  | 4.9  |
| 25  | DC    | 160  | TYR  | 4.9  |
| 27  | DE    | 147  | LEU  | 4.9  |
| 5   | AF    | 41   | ASP  | 4.9  |
| 25  | BC    | 178  | GLY  | 4.8  |
| 36  | DO    | 66   | GLY  | 4.8  |
| 51  | D4    | 8    | LYS  | 4.8  |
| 43  | BW    | 19   | ARG  | 4.8  |
| 42  | DU    | 76   | THR  | 4.8  |
| 43  | BW    | 42   | THR  | 4.8  |
| 25  | DC    | 29   | PHE  | 4.8  |
| 48  | D1    | 41   | VAL  | 4.8  |
| 15  | CP    | 52   | LEU  | 4.8  |
| 27  | DE    | 79   | ARG  | 4.8  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 41  | DT    | 69   | ARG  | 4.8  |
| 48  | B1    | 3    | GLY  | 4.8  |
| 31  | DJ    | 135  | GLN  | 4.8  |
| 26  | BD    | 91   | THR  | 4.8  |
| 23  | BB    | 1210 | G    | 4.8  |
| 23  | DB    | 1099 | G    | 4.8  |
| 25  | DC    | 10   | PRO  | 4.8  |
| 27  | DE    | 163  | ASN  | 4.8  |
| 45  | DY    | 10   | ARG  | 4.8  |
| 3   | CD    | 49   | ASP  | 4.8  |
| 11  | AL    | 69   | GLU  | 4.8  |
| 35  | DN    | 9    | GLN  | 4.8  |
| 39  | DR    | 86   | GLN  | 4.8  |
| 23  | BB    | 654  | A    | 4.8  |
| 26  | DD    | 16   | THR  | 4.8  |
| 29  | DG    | 170  | THR  | 4.8  |
| 33  | DL    | 12   | SER  | 4.8  |
| 41  | BT    | 27   | SER  | 4.8  |
| 49  | D2    | 45   | SER  | 4.8  |
| 34  | BM    | 95   | LEU  | 4.8  |
| 32  | BK    | 20   | MET  | 4.8  |
| 32  | BK    | 67   | LYS  | 4.8  |
| 50  | D3    | 46   | LYS  | 4.8  |
| 26  | DD    | 13   | ARG  | 4.8  |
| 37  | DP    | 33   | GLU  | 4.8  |
| 26  | DD    | 54   | ALA  | 4.8  |
| 29  | DG    | 173  | ALA  | 4.8  |
| 25  | BC    | 10   | PRO  | 4.8  |
| 30  | BH    | 11   | ASN  | 4.8  |
| 23  | DB    | 2309 | A    | 4.8  |
| 45  | BY    | 19   | HIS  | 4.8  |
| 32  | BK    | 38   | ILE  | 4.8  |
| 39  | BR    | 41   | ILE  | 4.8  |
| 39  | BR    | 37   | GLU  | 4.8  |
| 33  | BL    | 66   | PHE  | 4.8  |
| 26  | DD    | 9    | VAL  | 4.8  |
| 51  | B4    | 22   | VAL  | 4.8  |
| 16  | AQ    | 67   | SER  | 4.8  |
| 19  | AT    | 68   | LYS  | 4.8  |
| 25  | DC    | 39   | SER  | 4.8  |
| 26  | BD    | 145  | SER  | 4.8  |
| 2   | AC    | 158  | GLY  | 4.7  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | CA    | 412  | A    | 4.7  |
| 26  | DD    | 20   | VAL  | 4.7  |
| 27  | DE    | 173  | THR  | 4.7  |
| 49  | D2    | 22   | MET  | 4.7  |
| 43  | BW    | 8    | SER  | 4.7  |
| 12  | AM    | 104  | ASN  | 4.7  |
| 23  | DB    | 1459 | G    | 4.7  |
| 26  | DD    | 76   | GLY  | 4.7  |
| 24  | DV    | 56   | PHE  | 4.7  |
| 35  | BN    | 126  | ALA  | 4.7  |
| 41  | DT    | 56   | GLU  | 4.7  |
| 44  | DX    | 37   | LEU  | 4.7  |
| 44  | DX    | 47   | ARG  | 4.7  |
| 46  | DZ    | 21   | VAL  | 4.7  |
| 23  | BB    | 2799 | A    | 4.7  |
| 23  | DB    | 2799 | A    | 4.7  |
| 21  | AU    | 41   | THR  | 4.7  |
| 29  | DG    | 165  | ASP  | 4.7  |
| 42  | DU    | 88   | ASP  | 4.7  |
| 11  | AL    | 9    | LYS  | 4.7  |
| 36  | BO    | 3    | LYS  | 4.7  |
| 41  | BT    | 82   | LYS  | 4.7  |
| 31  | BJ    | 99   | ARG  | 4.7  |
| 32  | BK    | 78   | ARG  | 4.7  |
| 33  | DL    | 47   | ARG  | 4.7  |
| 38  | BQ    | 32   | ARG  | 4.7  |
| 28  | BF    | 83   | PRO  | 4.7  |
| 39  | BR    | 94   | THR  | 4.7  |
| 52  | BI    | 115  | ASP  | 4.7  |
| 23  | BB    | 1275 | A    | 4.7  |
| 38  | BQ    | 22   | GLY  | 4.7  |
| 50  | B3    | 24   | LYS  | 4.7  |
| 45  | BY    | 23   | LEU  | 4.7  |
| 26  | DD    | 68   | PHE  | 4.7  |
| 28  | BF    | 39   | VAL  | 4.7  |
| 25  | DC    | 172  | THR  | 4.7  |
| 42  | DU    | 14   | THR  | 4.7  |
| 37  | DP    | 110  | LYS  | 4.7  |
| 23  | DB    | 100  | U    | 4.7  |
| 8   | AI    | 34   | LEU  | 4.7  |
| 19  | AT    | 9    | ARG  | 4.7  |
| 25  | BC    | 211  | ARG  | 4.7  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 35  | BN    | 98   | LEU  | 4.7  |
| 25  | BC    | 165  | ALA  | 4.7  |
| 50  | B3    | 48   | MET  | 4.7  |
| 39  | DR    | 37   | GLU  | 4.7  |
| 25  | DC    | 21   | PRO  | 4.6  |
| 34  | DM    | 92   | TRP  | 4.6  |
| 49  | B2    | 46   | LYS  | 4.6  |
| 28  | BF    | 45   | ASP  | 4.6  |
| 50  | B3    | 43   | LEU  | 4.6  |
| 38  | DQ    | 112  | ALA  | 4.6  |
| 23  | BB    | 919  | U    | 4.6  |
| 25  | DC    | 235  | GLU  | 4.6  |
| 38  | DQ    | 110  | GLU  | 4.6  |
| 31  | DJ    | 110  | PRO  | 4.6  |
| 23  | BB    | 13   | A    | 4.6  |
| 32  | DK    | 81   | GLY  | 4.6  |
| 26  | DD    | 155  | VAL  | 4.6  |
| 31  | DJ    | 44   | TYR  | 4.6  |
| 39  | BR    | 64   | VAL  | 4.6  |
| 43  | BW    | 44   | PHE  | 4.6  |
| 52  | DI    | 7    | TYR  | 4.6  |
| 27  | BE    | 51   | GLU  | 4.6  |
| 11  | AL    | 111  | GLN  | 4.6  |
| 33  | BL    | 29   | LYS  | 4.6  |
| 45  | DY    | 2    | LYS  | 4.6  |
| 18  | AS    | 2    | ARG  | 4.6  |
| 18  | AS    | 14   | LEU  | 4.6  |
| 37  | DP    | 75   | THR  | 4.6  |
| 38  | BQ    | 7    | VAL  | 4.6  |
| 4   | CE    | 115  | GLU  | 4.6  |
| 39  | BR    | 24   | LYS  | 4.6  |
| 50  | B3    | 1    | PRO  | 4.6  |
| 43  | DW    | 38   | ARG  | 4.6  |
| 23  | BB    | 2213 | U    | 4.6  |
| 10  | AK    | 119  | GLY  | 4.6  |
| 11  | CL    | 22   | ALA  | 4.6  |
| 49  | D2    | 18   | PHE  | 4.6  |
| 1   | AA    | 78   | A    | 4.6  |
| 1   | AA    | 729  | A    | 4.6  |
| 23  | BB    | 2336 | A    | 4.6  |
| 34  | BM    | 123  | LYS  | 4.6  |
| 38  | BQ    | 48   | ASP  | 4.6  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 44  | BX    | 4    | LYS  | 4.6  |
| 48  | B1    | 2    | LYS  | 4.6  |
| 23  | BB    | 1076 | C    | 4.6  |
| 45  | DY    | 37   | ARG  | 4.6  |
| 25  | BC    | 153  | LEU  | 4.6  |
| 36  | BO    | 48   | LEU  | 4.6  |
| 26  | DD    | 111  | GLY  | 4.6  |
| 31  | BJ    | 40   | HIS  | 4.6  |
| 3   | AD    | 7    | LYS  | 4.5  |
| 3   | CD    | 72   | ARG  | 4.5  |
| 7   | AH    | 74   | ILE  | 4.5  |
| 47  | D0    | 49   | ARG  | 4.5  |
| 12  | AM    | 95   | PRO  | 4.5  |
| 43  | BW    | 73   | PRO  | 4.5  |
| 12  | AM    | 79   | LEU  | 4.5  |
| 37  | DP    | 56   | SER  | 4.5  |
| 29  | DG    | 42   | VAL  | 4.5  |
| 31  | BJ    | 79   | GLY  | 4.5  |
| 32  | BK    | 122  | VAL  | 4.5  |
| 44  | BX    | 46   | VAL  | 4.5  |
| 46  | BZ    | 36   | VAL  | 4.5  |
| 10  | AK    | 66   | ALA  | 4.5  |
| 34  | DM    | 56   | ALA  | 4.5  |
| 25  | DC    | 42   | ARG  | 4.5  |
| 36  | DO    | 16   | ARG  | 4.5  |
| 16  | CQ    | 4    | ILE  | 4.5  |
| 35  | BN    | 100  | CYS  | 4.5  |
| 51  | D4    | 16   | ILE  | 4.5  |
| 26  | BD    | 113  | SER  | 4.5  |
| 28  | BF    | 148  | VAL  | 4.5  |
| 30  | BH    | 130  | VAL  | 4.5  |
| 42  | BU    | 86   | PHE  | 4.5  |
| 3   | AD    | 150  | LYS  | 4.5  |
| 7   | AH    | 55   | LYS  | 4.5  |
| 52  | DI    | 6    | ALA  | 4.5  |
| 33  | BL    | 117  | THR  | 4.5  |
| 49  | B2    | 43   | THR  | 4.5  |
| 23  | BB    | 1205 | A    | 4.5  |
| 26  | DD    | 134  | HIS  | 4.5  |
| 23  | DB    | 331  | C    | 4.5  |
| 31  | DJ    | 120  | ARG  | 4.5  |
| 35  | DN    | 2    | ARG  | 4.5  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | CA    | 481  | G    | 4.5  |
| 23  | BB    | 1062 | G    | 4.5  |
| 23  | DB    | 2157 | G    | 4.5  |
| 50  | B3    | 62   | PRO  | 4.5  |
| 39  | DR    | 45   | GLU  | 4.5  |
| 39  | DR    | 75   | VAL  | 4.5  |
| 26  | BD    | 101  | PHE  | 4.5  |
| 49  | D2    | 13   | ASN  | 4.5  |
| 35  | BN    | 36   | THR  | 4.5  |
| 36  | DO    | 35   | ILE  | 4.5  |
| 37  | BP    | 98   | TYR  | 4.5  |
| 23  | BB    | 1090 | A    | 4.5  |
| 33  | BL    | 136  | GLU  | 4.5  |
| 3   | AD    | 191  | SER  | 4.5  |
| 27  | BE    | 54   | GLY  | 4.5  |
| 33  | DL    | 40   | SER  | 4.5  |
| 34  | BM    | 32   | GLY  | 4.5  |
| 36  | DO    | 13   | ARG  | 4.5  |
| 10  | AK    | 118  | ASN  | 4.5  |
| 8   | AI    | 42   | THR  | 4.5  |
| 25  | DC    | 14   | HIS  | 4.5  |
| 40  | BS    | 66   | ILE  | 4.5  |
| 28  | BF    | 65   | LEU  | 4.5  |
| 52  | DI    | 53   | PRO  | 4.5  |
| 12  | AM    | 26   | LYS  | 4.5  |
| 52  | DI    | 2    | LYS  | 4.5  |
| 31  | BJ    | 31   | GLU  | 4.5  |
| 31  | BJ    | 100  | VAL  | 4.5  |
| 52  | BI    | 4    | VAL  | 4.5  |
| 18  | CS    | 36   | ARG  | 4.5  |
| 26  | BD    | 15   | PHE  | 4.5  |
| 26  | DD    | 150  | GLN  | 4.5  |
| 27  | DE    | 88   | ARG  | 4.5  |
| 42  | DU    | 94   | PHE  | 4.5  |
| 23  | BB    | 2104 | C    | 4.4  |
| 35  | BN    | 124  | ALA  | 4.4  |
| 25  | BC    | 172  | THR  | 4.4  |
| 27  | DE    | 134  | LEU  | 4.4  |
| 1   | CA    | 1043 | G    | 4.4  |
| 23  | DB    | 2308 | G    | 4.4  |
| 36  | DO    | 4    | LYS  | 4.4  |
| 42  | BU    | 54   | PRO  | 4.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 43  | DW    | 74   | LYS  | 4.4  |
| 46  | DZ    | 42   | PRO  | 4.4  |
| 51  | B4    | 18   | LYS  | 4.4  |
| 21  | CU    | 35   | GLU  | 4.4  |
| 35  | DN    | 69   | ARG  | 4.4  |
| 9   | AJ    | 38   | GLY  | 4.4  |
| 33  | BL    | 55   | MET  | 4.4  |
| 21  | CU    | 12   | ASP  | 4.4  |
| 25  | DC    | 167  | ASP  | 4.4  |
| 31  | DJ    | 15   | TRP  | 4.4  |
| 36  | BO    | 8    | ILE  | 4.4  |
| 4   | CE    | 130  | THR  | 4.4  |
| 19  | AT    | 8    | LYS  | 4.4  |
| 25  | DC    | 6    | LYS  | 4.4  |
| 42  | DU    | 43   | LYS  | 4.4  |
| 36  | DO    | 28   | VAL  | 4.4  |
| 41  | DT    | 53   | VAL  | 4.4  |
| 28  | BF    | 31   | GLU  | 4.4  |
| 8   | CI    | 116  | GLY  | 4.4  |
| 19  | CT    | 71   | ALA  | 4.4  |
| 36  | DO    | 37   | ALA  | 4.4  |
| 1   | CA    | 1033 | G    | 4.4  |
| 23  | BB    | 1154 | G    | 4.4  |
| 23  | BB    | 2319 | G    | 4.4  |
| 48  | D1    | 44   | GLN  | 4.4  |
| 50  | D3    | 43   | LEU  | 4.4  |
| 42  | BU    | 44   | HIS  | 4.4  |
| 25  | BC    | 47   | ARG  | 4.4  |
| 27  | BE    | 61   | ARG  | 4.4  |
| 31  | BJ    | 37   | ARG  | 4.4  |
| 16  | AQ    | 6    | THR  | 4.4  |
| 43  | BW    | 57   | THR  | 4.4  |
| 52  | BI    | 70   | THR  | 4.4  |
| 25  | DC    | 127  | ASN  | 4.4  |
| 20  | CB    | 220  | VAL  | 4.4  |
| 16  | AQ    | 25   | GLU  | 4.4  |
| 27  | DE    | 25   | GLU  | 4.4  |
| 43  | BW    | 64   | GLY  | 4.4  |
| 52  | DI    | 27   | LEU  | 4.4  |
| 21  | AU    | 4    | LYS  | 4.4  |
| 10  | CK    | 127  | ARG  | 4.4  |
| 25  | DC    | 47   | ARG  | 4.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 33  | BL    | 21   | ARG  | 4.4  |
| 34  | DM    | 16   | ARG  | 4.4  |
| 50  | B3    | 39   | ARG  | 4.4  |
| 31  | BJ    | 76   | HIS  | 4.4  |
| 11  | CL    | 19   | ASN  | 4.4  |
| 33  | DL    | 46   | VAL  | 4.4  |
| 34  | DM    | 26   | VAL  | 4.4  |
| 35  | BN    | 109  | PRO  | 4.4  |
| 36  | DO    | 32   | PRO  | 4.4  |
| 46  | DZ    | 60   | PHE  | 4.3  |
| 4   | CE    | 107  | GLY  | 4.3  |
| 28  | DF    | 31   | GLU  | 4.3  |
| 29  | BG    | 159  | LYS  | 4.3  |
| 29  | DG    | 176  | LYS  | 4.3  |
| 31  | DJ    | 2    | LYS  | 4.3  |
| 35  | BN    | 65   | LEU  | 4.3  |
| 50  | D3    | 56   | LEU  | 4.3  |
| 7   | AH    | 125  | ILE  | 4.3  |
| 52  | BI    | 58   | ILE  | 4.3  |
| 10  | CK    | 126  | ARG  | 4.3  |
| 23  | BB    | 1847 | A    | 4.3  |
| 23  | BB    | 1348 | C    | 4.3  |
| 7   | AH    | 4    | ASP  | 4.3  |
| 11  | CL    | 103  | CYS  | 4.3  |
| 20  | AB    | 13   | VAL  | 4.3  |
| 25  | DC    | 65   | ASP  | 4.3  |
| 46  | DZ    | 50   | ASP  | 4.3  |
| 28  | DF    | 72   | SER  | 4.3  |
| 50  | D3    | 48   | MET  | 4.3  |
| 11  | AL    | 12   | ALA  | 4.3  |
| 18  | CS    | 64   | GLU  | 4.3  |
| 31  | DJ    | 82   | GLY  | 4.3  |
| 33  | BL    | 76   | GLU  | 4.3  |
| 33  | DL    | 144  | GLU  | 4.3  |
| 44  | DX    | 48   | ARG  | 4.3  |
| 18  | AS    | 18   | VAL  | 4.3  |
| 25  | DC    | 140  | VAL  | 4.3  |
| 26  | DD    | 152  | PRO  | 4.3  |
| 34  | DM    | 82   | MET  | 4.3  |
| 35  | BN    | 21   | PHE  | 4.3  |
| 2   | AC    | 179  | ALA  | 4.3  |
| 3   | AD    | 155  | LYS  | 4.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 11  | CL    | 87   | LYS  | 4.3  |
| 18  | AS    | 30   | LEU  | 4.3  |
| 23  | BB    | 1057 | A    | 4.3  |
| 23  | DB    | 1156 | A    | 4.3  |
| 29  | DG    | 58   | ALA  | 4.3  |
| 44  | DX    | 44   | LYS  | 4.3  |
| 26  | BD    | 53   | GLY  | 4.3  |
| 43  | DW    | 7    | GLY  | 4.3  |
| 3   | AD    | 43   | ARG  | 4.3  |
| 3   | AD    | 151  | GLN  | 4.3  |
| 29  | DG    | 3    | VAL  | 4.3  |
| 15  | AP    | 39   | PHE  | 4.3  |
| 34  | BM    | 132  | THR  | 4.3  |
| 45  | BY    | 52   | PHE  | 4.3  |
| 45  | DY    | 52   | PHE  | 4.3  |
| 47  | D0    | 25   | THR  | 4.3  |
| 12  | AM    | 55   | LEU  | 4.3  |
| 25  | BC    | 154  | ALA  | 4.3  |
| 46  | DZ    | 35   | ASP  | 4.3  |
| 25  | BC    | 42   | ARG  | 4.3  |
| 31  | BJ    | 112  | GLY  | 4.3  |
| 33  | BL    | 126  | ARG  | 4.3  |
| 33  | DL    | 20   | GLY  | 4.3  |
| 38  | DQ    | 73   | ILE  | 4.3  |
| 1   | AA    | 86   | G    | 4.3  |
| 23  | BB    | 504  | A    | 4.3  |
| 23  | BB    | 1175 | A    | 4.3  |
| 23  | DB    | 504  | A    | 4.3  |
| 33  | BL    | 104  | GLN  | 4.3  |
| 34  | BM    | 57   | VAL  | 4.3  |
| 27  | BE    | 85   | PHE  | 4.3  |
| 40  | BS    | 1    | MET  | 4.3  |
| 12  | AM    | 88   | LEU  | 4.3  |
| 8   | AI    | 15   | ALA  | 4.3  |
| 40  | DS    | 84   | ARG  | 4.3  |
| 43  | DW    | 5    | ALA  | 4.3  |
| 37  | BP    | 3    | ILE  | 4.3  |
| 46  | BZ    | 19   | GLY  | 4.3  |
| 25  | DC    | 177  | SER  | 4.3  |
| 27  | BE    | 72   | SER  | 4.3  |
| 44  | DX    | 39   | GLN  | 4.3  |
| 3   | CD    | 66   | VAL  | 4.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 15  | CP    | 13   | LYS  | 4.2  |
| 31  | BJ    | 18   | VAL  | 4.3  |
| 45  | DY    | 18   | LYS  | 4.2  |
| 1   | AA    | 466  | A    | 4.2  |
| 3   | AD    | 197  | HIS  | 4.2  |
| 37  | DP    | 73   | PHE  | 4.2  |
| 49  | D2    | 16   | HIS  | 4.2  |
| 25  | DC    | 204  | LEU  | 4.2  |
| 36  | BO    | 18   | LEU  | 4.2  |
| 36  | DO    | 62   | LEU  | 4.2  |
| 13  | AN    | 52   | ARG  | 4.2  |
| 6   | AG    | 38   | ALA  | 4.2  |
| 31  | BJ    | 103  | ILE  | 4.2  |
| 31  | BJ    | 51   | GLY  | 4.2  |
| 26  | BD    | 136  | ASN  | 4.2  |
| 33  | BL    | 106  | GLU  | 4.2  |
| 42  | DU    | 7    | ASP  | 4.2  |
| 49  | B2    | 8    | SER  | 4.2  |
| 13  | CN    | 6    | LYS  | 4.2  |
| 39  | BR    | 73   | LYS  | 4.2  |
| 52  | BI    | 138  | VAL  | 4.2  |
| 43  | BW    | 78   | PHE  | 4.2  |
| 11  | CL    | 12   | ALA  | 4.2  |
| 34  | BM    | 126  | ILE  | 4.2  |
| 37  | DP    | 63   | ILE  | 4.2  |
| 33  | BL    | 30   | THR  | 4.2  |
| 12  | AM    | 85   | TYR  | 4.2  |
| 23  | DB    | 10   | A    | 4.2  |
| 23  | DB    | 1175 | A    | 4.2  |
| 1   | CA    | 266  | G    | 4.2  |
| 23  | BB    | 2153 | C    | 4.2  |
| 3   | CD    | 146  | GLU  | 4.2  |
| 27  | BE    | 127  | GLU  | 4.2  |
| 33  | DL    | 143  | GLU  | 4.2  |
| 7   | CH    | 89   | ASP  | 4.2  |
| 26  | BD    | 131  | ASP  | 4.2  |
| 38  | BQ    | 96   | ASP  | 4.2  |
| 42  | BU    | 91   | LYS  | 4.2  |
| 47  | D0    | 19   | ASP  | 4.2  |
| 7   | AH    | 73   | SER  | 4.2  |
| 34  | DM    | 135  | VAL  | 4.2  |
| 46  | BZ    | 21   | VAL  | 4.2  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 19  | CT    | 60   | GLN  | 4.2  |
| 3   | AD    | 4    | LEU  | 4.2  |
| 28  | DF    | 70   | ARG  | 4.2  |
| 40  | DS    | 23   | LEU  | 4.2  |
| 34  | BM    | 68   | PHE  | 4.2  |
| 26  | DD    | 132  | ALA  | 4.2  |
| 45  | BY    | 12   | ALA  | 4.2  |
| 50  | B3    | 58   | ILE  | 4.2  |
| 12  | AM    | 83   | GLY  | 4.2  |
| 4   | CE    | 127  | TYR  | 4.2  |
| 51  | D4    | 34   | LYS  | 4.2  |
| 13  | AN    | 9    | GLU  | 4.2  |
| 23  | DB    | 1395 | A    | 4.2  |
| 37  | DP    | 82   | SER  | 4.2  |
| 47  | B0    | 30   | ASP  | 4.2  |
| 33  | BL    | 78   | ARG  | 4.2  |
| 47  | B0    | 15   | ARG  | 4.2  |
| 26  | DD    | 164  | GLN  | 4.2  |
| 1   | AA    | 79   | G    | 4.2  |
| 38  | DQ    | 105  | PHE  | 4.2  |
| 42  | DU    | 95   | PHE  | 4.2  |
| 25  | BC    | 48   | ILE  | 4.2  |
| 26  | BD    | 61   | THR  | 4.2  |
| 34  | DM    | 134  | THR  | 4.2  |
| 42  | BU    | 3    | LYS  | 4.2  |
| 33  | BL    | 10   | GLU  | 4.2  |
| 34  | BM    | 101  | VAL  | 4.2  |
| 37  | BP    | 10   | GLU  | 4.2  |
| 17  | AR    | 72   | ARG  | 4.2  |
| 21  | AU    | 34   | ARG  | 4.2  |
| 48  | B1    | 41   | VAL  | 4.2  |
| 23  | BB    | 1458 | U    | 4.2  |
| 27  | BE    | 163  | ASN  | 4.2  |
| 41  | DT    | 59   | ASN  | 4.2  |
| 43  | DW    | 14   | ASP  | 4.2  |
| 32  | BK    | 39   | ILE  | 4.2  |
| 1   | CA    | 1042 | A    | 4.2  |
| 38  | BQ    | 20   | ALA  | 4.2  |
| 50  | D3    | 47   | ALA  | 4.2  |
| 21  | CU    | 53   | LYS  | 4.2  |
| 43  | BW    | 74   | LYS  | 4.2  |
| 34  | BM    | 42   | THR  | 4.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | AA    | 1241 | G    | 4.2  |
| 16  | AQ    | 45   | VAL  | 4.1  |
| 38  | DQ    | 7    | VAL  | 4.1  |
| 43  | DW    | 13   | ARG  | 4.2  |
| 7   | AH    | 110  | MET  | 4.1  |
| 52  | BI    | 124  | MET  | 4.1  |
| 46  | BZ    | 48   | GLN  | 4.1  |
| 31  | BJ    | 84   | ILE  | 4.1  |
| 41  | DT    | 13   | ALA  | 4.1  |
| 46  | BZ    | 24   | ILE  | 4.1  |
| 3   | AD    | 205  | LYS  | 4.1  |
| 22  | BA    | 87   | U    | 4.1  |
| 23  | BB    | 62   | U    | 4.1  |
| 25  | BC    | 246  | PRO  | 4.1  |
| 35  | BN    | 5    | LYS  | 4.1  |
| 50  | D3    | 1    | PRO  | 4.1  |
| 50  | D3    | 2    | LYS  | 4.1  |
| 52  | DI    | 84   | GLY  | 4.1  |
| 6   | CG    | 4    | ARG  | 4.1  |
| 38  | DQ    | 2    | ARG  | 4.1  |
| 46  | DZ    | 59   | ARG  | 4.1  |
| 50  | D3    | 12   | ARG  | 4.1  |
| 3   | AD    | 52   | VAL  | 4.1  |
| 12  | CM    | 59   | VAL  | 4.1  |
| 43  | BW    | 66   | VAL  | 4.1  |
| 13  | AN    | 5    | MET  | 4.1  |
| 52  | BI    | 116  | MET  | 4.1  |
| 13  | AN    | 20   | PHE  | 4.1  |
| 5   | CF    | 51   | ILE  | 4.1  |
| 32  | BK    | 77   | ILE  | 4.1  |
| 27  | BE    | 128  | ALA  | 4.1  |
| 27  | DE    | 95   | LYS  | 4.1  |
| 37  | BP    | 95   | LYS  | 4.1  |
| 42  | DU    | 8    | ASP  | 4.1  |
| 28  | BF    | 64   | PRO  | 4.1  |
| 25  | BC    | 5    | CYS  | 4.1  |
| 25  | DC    | 51   | ARG  | 4.1  |
| 23  | BB    | 139  | U    | 4.1  |
| 23  | DB    | 2585 | U    | 4.1  |
| 25  | DC    | 139  | THR  | 4.1  |
| 47  | D0    | 53   | VAL  | 4.1  |
| 25  | BC    | 204  | LEU  | 4.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 44  | BX    | 14   | LEU  | 4.1  |
| 44  | DX    | 43   | LEU  | 4.1  |
| 1   | AA    | 74   | A    | 4.1  |
| 23  | DB    | 2406 | A    | 4.1  |
| 25  | DC    | 255  | LYS  | 4.1  |
| 51  | B4    | 26   | ILE  | 4.1  |
| 52  | DI    | 83   | ALA  | 4.1  |
| 48  | D1    | 30   | PRO  | 4.1  |
| 7   | CH    | 78   | SER  | 4.1  |
| 20  | AB    | 109  | SER  | 4.1  |
| 25  | BC    | 202  | ARG  | 4.1  |
| 32  | BK    | 80   | ASP  | 4.1  |
| 48  | B1    | 18   | HIS  | 4.1  |
| 3   | AD    | 5    | GLY  | 4.1  |
| 33  | BL    | 53   | GLY  | 4.1  |
| 1   | AA    | 765  | G    | 4.1  |
| 26  | BD    | 98   | VAL  | 4.1  |
| 27  | DE    | 112  | LEU  | 4.1  |
| 23  | BB    | 546  | U    | 4.1  |
| 23  | DB    | 2213 | U    | 4.1  |
| 27  | BE    | 57   | LYS  | 4.1  |
| 48  | B1    | 6    | GLU  | 4.1  |
| 2   | AC    | 159  | ALA  | 4.1  |
| 33  | DL    | 54   | GLN  | 4.1  |
| 3   | AD    | 145  | ARG  | 4.1  |
| 15  | CP    | 51   | ARG  | 4.1  |
| 52  | DI    | 21   | PRO  | 4.1  |
| 13  | CN    | 61   | ASN  | 4.1  |
| 23  | BB    | 508  | A    | 4.1  |
| 27  | BE    | 38   | GLY  | 4.1  |
| 48  | D1    | 18   | HIS  | 4.1  |
| 1   | CA    | 999  | C    | 4.1  |
| 3   | AD    | 20   | LEU  | 4.1  |
| 29  | BG    | 3    | VAL  | 4.1  |
| 33  | DL    | 61   | LEU  | 4.1  |
| 47  | B0    | 2    | VAL  | 4.1  |
| 2   | CC    | 191  | THR  | 4.1  |
| 45  | DY    | 20   | LYS  | 4.1  |
| 39  | BR    | 98   | ILE  | 4.1  |
| 32  | DK    | 49   | ARG  | 4.1  |
| 27  | DE    | 54   | GLY  | 4.1  |
| 39  | BR    | 89   | HIS  | 4.1  |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 49         | B2           | 17         | GLY         | 4.1         |
| 24         | DV           | 77         | VAL         | 4.0         |
| 26         | BD           | 178        | VAL         | 4.0         |
| 28         | DF           | 148        | VAL         | 4.0         |
| 2          | AC           | 153        | SER         | 4.0         |
| 31         | BJ           | 49         | ASP         | 4.0         |
| 13         | CN           | 46         | LYS         | 4.0         |
| 27         | DE           | 188        | MET         | 4.0         |
| 28         | BF           | 129        | MET         | 4.0         |
| 6          | AG           | 84         | TYR         | 4.0         |
| 25         | BC           | 8          | THR         | 4.0         |
| 31         | BJ           | 53         | TYR         | 4.0         |
| 20         | AB           | 39         | ILE         | 4.0         |
| 22         | BA           | 118        | C           | 4.0         |
| 21         | CU           | 46         | ARG         | 4.0         |
| 25         | DC           | 250        | GLN         | 4.0         |
| 15         | AP           | 74         | LEU         | 4.0         |
| 23         | BB           | 2320       | U           | 4.0         |
| 23         | DB           | 646        | U           | 4.0         |
| 23         | DB           | 846        | U           | 4.0         |
| 25         | DC           | 164        | VAL         | 4.0         |
| 31         | DJ           | 62         | VAL         | 4.0         |
| 1          | AA           | 126        | G           | 4.0         |
| 1          | CA           | 993        | G           | 4.0         |
| 21         | AU           | 24         | LYS         | 4.0         |
| 31         | DJ           | 85         | LYS         | 4.0         |
| 33         | DL           | 14         | LYS         | 4.0         |
| 8          | CI           | 37         | TYR         | 4.0         |
| 25         | BC           | 266        | ILE         | 4.0         |
| 26         | DD           | 2          | ILE         | 4.0         |
| 26         | DD           | 22         | ILE         | 4.0         |
| 38         | DQ           | 93         | ILE         | 4.0         |
| 25         | BC           | 166        | ARG         | 4.0         |
| 48         | D1           | 43         | ARG         | 4.0         |
| 7          | CH           | 7          | ALA         | 4.0         |
| 18         | CS           | 74         | ALA         | 4.0         |
| 39         | BR           | 45         | GLU         | 4.0         |
| 41         | BT           | 25         | GLU         | 4.0         |
| 42         | BU           | 87         | GLU         | 4.0         |
| 45         | BY           | 49         | ALA         | 4.0         |
| 1          | AA           | 65         | A           | 4.0         |
| 1          | CA           | 975        | A           | 4.0         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 14  | AO    | 39  | GLN  | 4.0  |
| 21  | CU    | 28  | LEU  | 4.0  |
| 3   | CD    | 150 | LYS  | 4.0  |
| 30  | DH    | 19  | VAL  | 4.0  |
| 47  | B0    | 53  | VAL  | 4.0  |
| 18  | CS    | 65  | MET  | 4.0  |
| 25  | BC    | 225 | ASN  | 4.0  |
| 16  | AQ    | 26  | ARG  | 4.0  |
| 36  | DO    | 2   | ASP  | 4.0  |
| 42  | BU    | 71  | ILE  | 4.0  |
| 50  | D3    | 29  | ARG  | 4.0  |
| 26  | DD    | 133 | THR  | 4.0  |
| 46  | DZ    | 13  | THR  | 4.0  |
| 2   | CC    | 70  | ALA  | 4.0  |
| 23  | DB    | 411 | G    | 4.0  |
| 14  | AO    | 55  | LEU  | 4.0  |
| 14  | CO    | 61  | GLN  | 4.0  |
| 19  | CT    | 68  | LYS  | 4.0  |
| 26  | BD    | 55  | LYS  | 4.0  |
| 27  | DE    | 90  | GLN  | 4.0  |
| 36  | BO    | 42  | PRO  | 4.0  |
| 37  | DP    | 74  | GLN  | 4.0  |
| 27  | BE    | 42  | GLY  | 4.0  |
| 33  | DL    | 34  | GLY  | 4.0  |
| 36  | BO    | 103 | VAL  | 4.0  |
| 43  | BW    | 50  | VAL  | 4.0  |
| 50  | B3    | 46  | LYS  | 4.0  |
| 1   | AA    | 728 | A    | 4.0  |
| 43  | BW    | 2   | HIS  | 4.0  |
| 47  | B0    | 14  | MET  | 4.0  |
| 38  | BQ    | 10  | ARG  | 4.0  |
| 43  | DW    | 40  | ARG  | 4.0  |
| 26  | DD    | 12  | THR  | 4.0  |
| 27  | DE    | 39  | ALA  | 4.0  |
| 9   | AJ    | 52  | LEU  | 4.0  |
| 11  | CL    | 9   | LYS  | 4.0  |
| 13  | CN    | 45  | LEU  | 4.0  |
| 28  | BF    | 116 | LEU  | 4.0  |
| 29  | BG    | 153 | PRO  | 4.0  |
| 30  | DH    | 78  | VAL  | 4.0  |
| 52  | BI    | 57  | VAL  | 4.0  |
| 33  | BL    | 11  | GLY  | 4.0  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 8   | CI    | 123  | ARG  | 4.0  |
| 11  | AL    | 8    | ARG  | 4.0  |
| 18  | CS    | 33   | TRP  | 4.0  |
| 23  | DB    | 1401 | G    | 4.0  |
| 36  | DO    | 92   | PHE  | 4.0  |
| 23  | DB    | 2602 | A    | 4.0  |
| 25  | DC    | 238  | ASN  | 4.0  |
| 37  | DP    | 57   | ALA  | 4.0  |
| 38  | DQ    | 95   | ALA  | 4.0  |
| 36  | BO    | 53   | THR  | 4.0  |
| 21  | CU    | 43   | GLU  | 4.0  |
| 38  | BQ    | 88   | GLU  | 4.0  |
| 20  | CB    | 56   | LEU  | 4.0  |
| 42  | BU    | 40   | LEU  | 4.0  |
| 44  | BX    | 44   | LYS  | 4.0  |
| 52  | BI    | 2    | LYS  | 4.0  |
| 10  | AK    | 53   | GLY  | 3.9  |
| 41  | DT    | 91   | GLN  | 3.9  |
| 6   | AG    | 3    | ARG  | 3.9  |
| 21  | AU    | 32   | ARG  | 3.9  |
| 36  | DO    | 30   | ARG  | 3.9  |
| 43  | DW    | 24   | ARG  | 3.9  |
| 51  | D4    | 27   | CYS  | 3.9  |
| 37  | BP    | 55   | HIS  | 3.9  |
| 26  | BD    | 2    | ILE  | 3.9  |
| 26  | BD    | 27   | ILE  | 3.9  |
| 44  | BX    | 26   | PHE  | 3.9  |
| 25  | BC    | 30   | ALA  | 3.9  |
| 38  | DQ    | 117  | ALA  | 3.9  |
| 40  | DS    | 10   | ALA  | 3.9  |
| 25  | DC    | 38   | LYS  | 3.9  |
| 20  | AB    | 211  | LEU  | 3.9  |
| 35  | DN    | 10   | LEU  | 3.9  |
| 11  | AL    | 24   | GLU  | 3.9  |
| 23  | BB    | 1699 | G    | 3.9  |
| 29  | DG    | 1    | SER  | 3.9  |
| 31  | BJ    | 9    | GLU  | 3.9  |
| 46  | BZ    | 11   | GLU  | 3.9  |
| 23  | BB    | 2406 | A    | 3.9  |
| 21  | CU    | 32   | ARG  | 3.9  |
| 30  | DH    | 123  | ARG  | 3.9  |
| 47  | B0    | 7    | PRO  | 3.9  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 47  | D0    | 34   | GLY  | 3.9  |
| 38  | BQ    | 43   | GLN  | 3.9  |
| 14  | CO    | 37   | HIS  | 3.9  |
| 17  | CR    | 58   | ILE  | 3.9  |
| 23  | BB    | 2491 | U    | 3.9  |
| 23  | DB    | 1460 | U    | 3.9  |
| 47  | D0    | 56   | LYS  | 3.9  |
| 40  | DS    | 45   | VAL  | 3.9  |
| 41  | BT    | 10   | VAL  | 3.9  |
| 27  | BE    | 171  | ASP  | 3.9  |
| 28  | BF    | 152  | ASP  | 3.9  |
| 47  | D0    | 15   | ARG  | 3.9  |
| 26  | DD    | 23   | PRO  | 3.9  |
| 1   | AA    | 1441 | A    | 3.9  |
| 23  | BB    | 1086 | A    | 3.9  |
| 29  | DG    | 23   | ILE  | 3.9  |
| 31  | DJ    | 40   | HIS  | 3.9  |
| 39  | DR    | 81   | LYS  | 3.9  |
| 7   | CH    | 62   | LEU  | 3.9  |
| 36  | BO    | 70   | ALA  | 3.9  |
| 23  | DB    | 1217 | U    | 3.9  |
| 8   | CI    | 110  | VAL  | 3.9  |
| 11  | CL    | 93   | ARG  | 3.9  |
| 13  | CN    | 33   | VAL  | 3.9  |
| 19  | AT    | 28   | ARG  | 3.9  |
| 26  | BD    | 52   | THR  | 3.9  |
| 26  | BD    | 92   | VAL  | 3.9  |
| 31  | DJ    | 43   | GLU  | 3.9  |
| 35  | DN    | 46   | ARG  | 3.9  |
| 41  | BT    | 69   | ARG  | 3.9  |
| 19  | AT    | 2    | ASN  | 3.9  |
| 9   | CJ    | 60   | ASP  | 3.9  |
| 32  | DK    | 14   | SER  | 3.9  |
| 40  | BS    | 79   | GLY  | 3.9  |
| 52  | BI    | 118  | GLY  | 3.9  |
| 25  | BC    | 162  | GLN  | 3.9  |
| 25  | DC    | 63   | ILE  | 3.9  |
| 5   | CF    | 80   | PHE  | 3.9  |
| 11  | AL    | 87   | LYS  | 3.9  |
| 25  | BC    | 169  | ALA  | 3.9  |
| 27  | DE    | 138  | LEU  | 3.9  |
| 28  | BF    | 151  | LEU  | 3.9  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 41  | DT    | 7    | LEU  | 3.9  |
| 23  | BB    | 2211 | A    | 3.9  |
| 34  | DM    | 40   | ARG  | 3.9  |
| 39  | DR    | 84   | ARG  | 3.9  |
| 41  | BT    | 6    | ARG  | 3.9  |
| 1   | AA    | 108  | G    | 3.9  |
| 1   | AA    | 550  | G    | 3.9  |
| 1   | CA    | 372  | C    | 3.9  |
| 30  | DH    | 115  | VAL  | 3.9  |
| 27  | BE    | 111  | GLU  | 3.9  |
| 48  | D1    | 16   | THR  | 3.9  |
| 18  | CS    | 25   | GLY  | 3.9  |
| 25  | BC    | 126  | GLY  | 3.9  |
| 52  | BI    | 53   | PRO  | 3.9  |
| 9   | CJ    | 76   | ILE  | 3.9  |
| 17  | AR    | 38   | ILE  | 3.9  |
| 26  | DD    | 159  | LYS  | 3.9  |
| 28  | DF    | 84   | ILE  | 3.9  |
| 52  | DI    | 80   | LYS  | 3.9  |
| 13  | CN    | 70   | HIS  | 3.9  |
| 27  | DE    | 165  | HIS  | 3.9  |
| 50  | D3    | 30   | HIS  | 3.9  |
| 7   | CH    | 129  | ALA  | 3.9  |
| 49  | D2    | 33   | ARG  | 3.8  |
| 27  | DE    | 120  | VAL  | 3.8  |
| 8   | CI    | 111  | GLU  | 3.8  |
| 11  | CL    | 37   | TYR  | 3.8  |
| 16  | AQ    | 62   | GLU  | 3.8  |
| 17  | AR    | 19   | GLU  | 3.8  |
| 26  | BD    | 11   | MET  | 3.8  |
| 26  | DD    | 91   | THR  | 3.8  |
| 29  | BG    | 170  | THR  | 3.8  |
| 9   | CJ    | 43   | PRO  | 3.8  |
| 23  | DB    | 2135 | A    | 3.8  |
| 12  | CM    | 3    | ILE  | 3.8  |
| 25  | DC    | 48   | ILE  | 3.8  |
| 42  | DU    | 34   | ILE  | 3.8  |
| 1   | AA    | 5    | U    | 3.8  |
| 23  | DB    | 392  | U    | 3.8  |
| 42  | BU    | 45   | GLN  | 3.8  |
| 14  | CO    | 45   | HIS  | 3.8  |
| 37  | DP    | 92   | ARG  | 3.8  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 48  | B1    | 1    | ALA  | 3.8  |
| 4   | AE    | 113  | VAL  | 3.8  |
| 29  | DG    | 167  | VAL  | 3.8  |
| 42  | BU    | 82   | VAL  | 3.8  |
| 52  | DI    | 4    | VAL  | 3.8  |
| 30  | BH    | 22   | LYS  | 3.8  |
| 38  | BQ    | 4    | LYS  | 3.8  |
| 36  | DO    | 31   | THR  | 3.8  |
| 37  | DP    | 47   | ILE  | 3.8  |
| 28  | DF    | 174  | PHE  | 3.8  |
| 37  | BP    | 51   | ASN  | 3.8  |
| 8   | CI    | 109  | GLN  | 3.8  |
| 9   | CJ    | 87   | LEU  | 3.8  |
| 36  | DO    | 19   | GLN  | 3.8  |
| 1   | CA    | 532  | A    | 3.8  |
| 19  | AT    | 13   | SER  | 3.8  |
| 33  | BL    | 41   | ARG  | 3.8  |
| 34  | BM    | 18   | ARG  | 3.8  |
| 35  | BN    | 19   | ALA  | 3.8  |
| 42  | BU    | 63   | ALA  | 3.8  |
| 1   | AA    | 632  | U    | 3.8  |
| 37  | DP    | 16   | VAL  | 3.8  |
| 3   | AD    | 147  | LYS  | 3.8  |
| 21  | CU    | 45   | LYS  | 3.8  |
| 37  | DP    | 28   | LYS  | 3.8  |
| 49  | D2    | 11   | LYS  | 3.8  |
| 8   | AI    | 64   | ILE  | 3.8  |
| 34  | BM    | 65   | ILE  | 3.8  |
| 38  | BQ    | 25   | GLY  | 3.8  |
| 39  | DR    | 98   | ILE  | 3.8  |
| 8   | CI    | 83   | THR  | 3.8  |
| 12  | CM    | 104  | ASN  | 3.8  |
| 25  | BC    | 89   | ASN  | 3.8  |
| 30  | BH    | 20   | ASN  | 3.8  |
| 14  | AO    | 34   | GLN  | 3.8  |
| 26  | BD    | 162  | ALA  | 3.8  |
| 37  | BP    | 35   | SER  | 3.8  |
| 20  | CB    | 162  | VAL  | 3.8  |
| 9   | AJ    | 59   | LYS  | 3.8  |
| 11  | AL    | 122  | LYS  | 3.8  |
| 30  | DH    | 112  | LYS  | 3.8  |
| 23  | BB    | 2602 | A    | 3.8  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | AA    | 789  | U    | 3.8  |
| 1   | CA    | 632  | U    | 3.8  |
| 1   | CA    | 970  | C    | 3.8  |
| 3   | CD    | 203  | TYR  | 3.8  |
| 25  | BC    | 137  | GLY  | 3.8  |
| 51  | D4    | 21   | GLY  | 3.8  |
| 25  | BC    | 86   | ARG  | 3.8  |
| 33  | BL    | 94   | THR  | 3.8  |
| 34  | BM    | 31   | PHE  | 3.8  |
| 34  | DM    | 38   | ARG  | 3.8  |
| 50  | B3    | 41   | ARG  | 3.8  |
| 51  | B4    | 19   | ARG  | 3.8  |
| 23  | BB    | 1055 | G    | 3.8  |
| 13  | AN    | 48   | GLN  | 3.8  |
| 41  | BT    | 72   | GLN  | 3.8  |
| 52  | DI    | 132  | ALA  | 3.8  |
| 3   | AD    | 82   | LYS  | 3.8  |
| 8   | CI    | 13   | SER  | 3.8  |
| 14  | AO    | 72   | LYS  | 3.8  |
| 26  | BD    | 157  | LYS  | 3.8  |
| 29  | BG    | 91   | VAL  | 3.8  |
| 31  | DJ    | 18   | VAL  | 3.8  |
| 49  | B2    | 37   | LYS  | 3.8  |
| 51  | D4    | 15   | LYS  | 3.8  |
| 52  | BI    | 8    | VAL  | 3.8  |
| 28  | DF    | 55   | ASP  | 3.8  |
| 38  | BQ    | 60   | TRP  | 3.8  |
| 8   | CI    | 56   | MET  | 3.8  |
| 41  | DT    | 2    | ILE  | 3.8  |
| 3   | AD    | 62   | ARG  | 3.8  |
| 25  | DC    | 214  | GLY  | 3.8  |
| 33  | DL    | 51   | GLU  | 3.8  |
| 35  | DN    | 123  | GLU  | 3.8  |
| 1   | AA    | 1493 | A    | 3.8  |
| 26  | BD    | 112  | THR  | 3.8  |
| 1   | AA    | 307  | C    | 3.7  |
| 1   | AA    | 578  | C    | 3.7  |
| 25  | DC    | 30   | ALA  | 3.7  |
| 38  | BQ    | 117  | ALA  | 3.7  |
| 26  | BD    | 154  | LYS  | 3.7  |
| 41  | BT    | 66   | LYS  | 3.7  |
| 15  | AP    | 9    | HIS  | 3.7  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 13  | CN    | 5    | MET  | 3.7  |
| 1   | AA    | 164  | G    | 3.7  |
| 1   | CA    | 31   | G    | 3.7  |
| 23  | BB    | 2808 | G    | 3.7  |
| 23  | DB    | 2156 | G    | 3.7  |
| 19  | AT    | 23   | ARG  | 3.7  |
| 37  | BP    | 61   | ARG  | 3.7  |
| 26  | DD    | 138  | LEU  | 3.7  |
| 33  | DL    | 140  | GLY  | 3.7  |
| 43  | BW    | 58   | LEU  | 3.7  |
| 3   | AD    | 34   | GLU  | 3.7  |
| 16  | CQ    | 27   | PHE  | 3.7  |
| 39  | DR    | 93   | PHE  | 3.7  |
| 46  | BZ    | 43   | PHE  | 3.7  |
| 25  | DC    | 190  | THR  | 3.7  |
| 30  | BH    | 124  | THR  | 3.7  |
| 16  | CQ    | 38   | LYS  | 3.7  |
| 33  | DL    | 29   | LYS  | 3.7  |
| 34  | DM    | 76   | LYS  | 3.7  |
| 23  | BB    | 1058 | U    | 3.7  |
| 30  | BH    | 19   | VAL  | 3.7  |
| 36  | DO    | 103  | VAL  | 3.7  |
| 23  | BB    | 1808 | A    | 3.7  |
| 23  | BB    | 2154 | A    | 3.7  |
| 16  | AQ    | 44   | HIS  | 3.7  |
| 34  | BM    | 17   | ASN  | 3.7  |
| 19  | AT    | 27   | MET  | 3.7  |
| 23  | DB    | 1100 | C    | 3.7  |
| 28  | BF    | 140  | ILE  | 3.7  |
| 33  | DL    | 18   | ARG  | 3.7  |
| 46  | DZ    | 5    | ILE  | 3.7  |
| 26  | BD    | 103  | ASP  | 3.7  |
| 47  | D0    | 45   | ASP  | 3.7  |
| 28  | DF    | 15   | LEU  | 3.7  |
| 11  | CL    | 90   | PRO  | 3.7  |
| 40  | BS    | 75   | PHE  | 3.7  |
| 7   | AH    | 64   | TYR  | 3.7  |
| 14  | CO    | 44   | GLU  | 3.7  |
| 35  | BN    | 43   | GLU  | 3.7  |
| 34  | BM    | 100  | LYS  | 3.7  |
| 51  | B4    | 5    | ALA  | 3.7  |
| 25  | DC    | 93   | VAL  | 3.7  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 31  | DJ    | 13   | ARG  | 3.7  |
| 36  | DO    | 33   | ARG  | 3.7  |
| 42  | BU    | 39   | ASN  | 3.7  |
| 49  | D2    | 34   | ARG  | 3.7  |
| 50  | D3    | 31   | ILE  | 3.7  |
| 36  | BO    | 21   | LEU  | 3.7  |
| 13  | AN    | 71   | GLY  | 3.7  |
| 27  | DE    | 184  | ASP  | 3.7  |
| 29  | BG    | 160  | GLY  | 3.7  |
| 38  | DQ    | 42   | GLY  | 3.7  |
| 1   | CA    | 381  | C    | 3.7  |
| 10  | CK    | 90   | PRO  | 3.7  |
| 5   | CF    | 53   | LYS  | 3.7  |
| 18  | CS    | 69   | LYS  | 3.7  |
| 20  | AB    | 27   | LYS  | 3.7  |
| 23  | BB    | 1102 | C    | 3.7  |
| 6   | AG    | 73   | GLU  | 3.7  |
| 39  | BR    | 71   | LYS  | 3.7  |
| 46  | DZ    | 8    | LYS  | 3.7  |
| 52  | BI    | 7    | TYR  | 3.7  |
| 14  | AO    | 33   | ALA  | 3.7  |
| 47  | D0    | 43   | THR  | 3.7  |
| 52  | BI    | 6    | ALA  | 3.7  |
| 26  | BD    | 170  | VAL  | 3.7  |
| 36  | BO    | 47   | VAL  | 3.7  |
| 16  | CQ    | 26   | ARG  | 3.7  |
| 43  | DW    | 2    | HIS  | 3.7  |
| 19  | AT    | 38   | ILE  | 3.7  |
| 1   | CA    | 1174 | G    | 3.7  |
| 20  | AB    | 128  | LEU  | 3.7  |
| 7   | AH    | 122  | GLY  | 3.7  |
| 19  | AT    | 70   | LYS  | 3.7  |
| 33  | BL    | 65   | GLY  | 3.7  |
| 42  | BU    | 31   | GLY  | 3.7  |
| 43  | BW    | 77   | LYS  | 3.7  |
| 44  | BX    | 62   | GLY  | 3.7  |
| 48  | D1    | 38   | PHE  | 3.7  |
| 3   | CD    | 37   | PRO  | 3.7  |
| 7   | AH    | 104  | SER  | 3.7  |
| 23  | DB    | 390  | U    | 3.7  |
| 37  | DP    | 77   | SER  | 3.7  |
| 25  | BC    | 179  | GLU  | 3.7  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 27  | BE    | 2    | GLU  | 3.7  |
| 35  | BN    | 94   | TYR  | 3.7  |
| 13  | CN    | 98   | ALA  | 3.7  |
| 27  | BE    | 160  | ALA  | 3.7  |
| 33  | BL    | 98   | ALA  | 3.7  |
| 43  | DW    | 48   | ALA  | 3.7  |
| 44  | DX    | 32   | ALA  | 3.7  |
| 8   | AI    | 18   | VAL  | 3.7  |
| 19  | CT    | 57   | VAL  | 3.7  |
| 34  | BM    | 131  | VAL  | 3.7  |
| 41  | DT    | 31   | VAL  | 3.7  |
| 41  | DT    | 58   | VAL  | 3.7  |
| 1   | AA    | 217  | C    | 3.7  |
| 1   | AA    | 372  | C    | 3.7  |
| 1   | AA    | 1317 | C    | 3.7  |
| 1   | CA    | 1400 | C    | 3.7  |
| 27  | BE    | 69   | ARG  | 3.7  |
| 47  | D0    | 16   | ARG  | 3.7  |
| 27  | BE    | 199  | MET  | 3.7  |
| 42  | DU    | 65   | GLN  | 3.7  |
| 2   | CC    | 74   | ILE  | 3.7  |
| 5   | AF    | 6    | ILE  | 3.7  |
| 25  | DC    | 52   | HIS  | 3.7  |
| 39  | BR    | 22   | LEU  | 3.7  |
| 43  | BW    | 43   | LYS  | 3.7  |
| 10  | AK    | 87   | GLY  | 3.7  |
| 18  | CS    | 7    | GLY  | 3.7  |
| 35  | BN    | 101  | GLY  | 3.7  |
| 35  | DN    | 87   | PHE  | 3.7  |
| 2   | CC    | 165  | GLU  | 3.6  |
| 4   | AE    | 21   | SER  | 3.6  |
| 5   | CF    | 100  | SER  | 3.6  |
| 47  | B0    | 28   | SER  | 3.6  |
| 1   | AA    | 220  | G    | 3.6  |
| 8   | CI    | 6    | TYR  | 3.6  |
| 20  | AB    | 74   | ALA  | 3.6  |
| 21  | AU    | 25   | ALA  | 3.6  |
| 23  | DB    | 2107 | G    | 3.6  |
| 30  | BH    | 36   | ALA  | 3.6  |
| 34  | DM    | 70   | ASP  | 3.6  |
| 36  | BO    | 64   | TYR  | 3.6  |
| 39  | BR    | 83   | TYR  | 3.6  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 5   | CF    | 86   | ARG  | 3.6  |
| 33  | DL    | 33   | ARG  | 3.6  |
| 45  | DY    | 30   | ARG  | 3.6  |
| 52  | BI    | 125  | THR  | 3.6  |
| 51  | B4    | 37   | GLN  | 3.6  |
| 36  | DO    | 34   | HIS  | 3.6  |
| 37  | BP    | 13   | LYS  | 3.6  |
| 1   | AA    | 135  | C    | 3.6  |
| 27  | DE    | 60   | TRP  | 3.6  |
| 31  | BJ    | 33   | ALA  | 3.6  |
| 36  | DO    | 9    | ARG  | 3.6  |
| 41  | DT    | 54   | GLU  | 3.6  |
| 46  | BZ    | 56   | ARG  | 3.6  |
| 46  | DZ    | 28   | VAL  | 3.6  |
| 4   | AE    | 89   | THR  | 3.6  |
| 31  | BJ    | 1    | MET  | 3.6  |
| 5   | AF    | 51   | ILE  | 3.6  |
| 1   | CA    | 467  | U    | 3.6  |
| 23  | BB    | 34   | U    | 3.6  |
| 33  | DL    | 17   | LYS  | 3.6  |
| 38  | BQ    | 92   | LYS  | 3.6  |
| 43  | DW    | 23   | LYS  | 3.6  |
| 23  | BB    | 1160 | G    | 3.6  |
| 29  | BG    | 51   | PHE  | 3.6  |
| 6   | CG    | 3    | ARG  | 3.6  |
| 13  | CN    | 44   | VAL  | 3.6  |
| 29  | BG    | 164  | ALA  | 3.6  |
| 27  | DE    | 55   | SER  | 3.6  |
| 42  | BU    | 97   | SER  | 3.6  |
| 19  | AT    | 63   | LYS  | 3.6  |
| 19  | CT    | 15   | LYS  | 3.6  |
| 36  | BO    | 31   | THR  | 3.6  |
| 36  | BO    | 106  | LEU  | 3.6  |
| 48  | D1    | 36   | LYS  | 3.6  |
| 52  | BI    | 10   | LEU  | 3.6  |
| 5   | CF    | 46   | GLN  | 3.6  |
| 30  | DH    | 33   | GLN  | 3.6  |
| 2   | CC    | 154  | GLY  | 3.6  |
| 23  | BB    | 2180 | U    | 3.6  |
| 42  | BU    | 37   | GLY  | 3.6  |
| 49  | D2    | 12   | ARG  | 3.6  |
| 8   | AI    | 124  | PRO  | 3.6  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 11  | AL    | 27   | PRO  | 3.6  |
| 2   | AC    | 136  | ALA  | 3.6  |
| 7   | AH    | 102  | VAL  | 3.6  |
| 39  | DR    | 33   | VAL  | 3.6  |
| 1   | AA    | 266  | G    | 3.6  |
| 1   | AA    | 377  | G    | 3.6  |
| 1   | CA    | 765  | G    | 3.6  |
| 38  | DQ    | 88   | GLU  | 3.6  |
| 1   | CA    | 747  | A    | 3.6  |
| 33  | BL    | 63   | LYS  | 3.6  |
| 33  | BL    | 96   | LYS  | 3.6  |
| 38  | BQ    | 46   | TYR  | 3.6  |
| 34  | DM    | 2    | LEU  | 3.6  |
| 43  | DW    | 18   | LYS  | 3.6  |
| 3   | CD    | 27   | ILE  | 3.6  |
| 37  | DP    | 1    | SER  | 3.6  |
| 26  | DD    | 36   | GLN  | 3.6  |
| 5   | CF    | 37   | HIS  | 3.6  |
| 6   | CG    | 7    | GLY  | 3.6  |
| 11  | AL    | 84   | GLY  | 3.6  |
| 42  | DU    | 31   | GLY  | 3.6  |
| 13  | CN    | 56   | PRO  | 3.6  |
| 25  | DC    | 171  | VAL  | 3.6  |
| 25  | DC    | 243  | PRO  | 3.6  |
| 31  | DJ    | 134  | ALA  | 3.6  |
| 43  | BW    | 70   | VAL  | 3.6  |
| 25  | BC    | 22   | GLU  | 3.6  |
| 26  | DD    | 55   | LYS  | 3.6  |
| 35  | DN    | 32   | GLU  | 3.6  |
| 35  | DN    | 127  | GLU  | 3.6  |
| 41  | DT    | 33   | LYS  | 3.6  |
| 49  | D2    | 42   | LEU  | 3.6  |
| 35  | DN    | 75   | ILE  | 3.6  |
| 40  | BS    | 85   | ILE  | 3.6  |
| 46  | BZ    | 17   | SER  | 3.6  |
| 1   | AA    | 461  | A    | 3.5  |
| 5   | CF    | 79   | ARG  | 3.5  |
| 20  | AB    | 94   | ARG  | 3.5  |
| 22  | DA    | 61   | G    | 3.5  |
| 23  | DB    | 2413 | G    | 3.5  |
| 5   | CF    | 94   | HIS  | 3.5  |
| 33  | DL    | 69   | ARG  | 3.5  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 37  | BP    | 71   | ARG  | 3.5  |
| 23  | BB    | 2146 | C    | 3.5  |
| 3   | AD    | 154  | VAL  | 3.5  |
| 34  | BM    | 93   | VAL  | 3.5  |
| 36  | DO    | 49   | VAL  | 3.5  |
| 42  | BU    | 69   | VAL  | 3.5  |
| 33  | BL    | 83   | ALA  | 3.5  |
| 43  | DW    | 17   | ALA  | 3.5  |
| 34  | DM    | 84   | LYS  | 3.5  |
| 48  | D1    | 37   | LYS  | 3.5  |
| 28  | BF    | 35   | LEU  | 3.5  |
| 33  | BL    | 1    | MET  | 3.5  |
| 35  | BN    | 10   | LEU  | 3.5  |
| 3   | AD    | 196  | GLU  | 3.5  |
| 4   | CE    | 100  | GLU  | 3.5  |
| 24  | BV    | 24   | ASN  | 3.5  |
| 40  | BS    | 59   | GLU  | 3.5  |
| 34  | DM    | 103  | TYR  | 3.5  |
| 26  | BD    | 77   | ARG  | 3.5  |
| 25  | DC    | 66   | PHE  | 3.5  |
| 26  | BD    | 139  | SER  | 3.5  |
| 34  | DM    | 7    | THR  | 3.5  |
| 36  | BO    | 117  | PHE  | 3.5  |
| 25  | BC    | 186  | ASP  | 3.5  |
| 25  | DC    | 116  | GLN  | 3.5  |
| 39  | BR    | 87   | GLN  | 3.5  |
| 45  | BY    | 14   | GLY  | 3.5  |
| 26  | DD    | 26   | VAL  | 3.5  |
| 34  | BM    | 86   | LYS  | 3.5  |
| 34  | DM    | 86   | LYS  | 3.5  |
| 37  | DP    | 72   | VAL  | 3.5  |
| 46  | BZ    | 47   | LYS  | 3.5  |
| 1   | CA    | 1493 | A    | 3.5  |
| 9   | AJ    | 42   | LEU  | 3.5  |
| 51  | D4    | 10   | LEU  | 3.5  |
| 23  | BB    | 1116 | G    | 3.5  |
| 23  | DB    | 51   | G    | 3.5  |
| 23  | DB    | 1055 | G    | 3.5  |
| 23  | DB    | 1537 | G    | 3.5  |
| 26  | DD    | 64   | GLU  | 3.5  |
| 26  | DD    | 146  | ILE  | 3.5  |
| 35  | DN    | 113  | ILE  | 3.5  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 19  | CT    | 51   | ASN  | 3.5  |
| 26  | BD    | 128  | ARG  | 3.5  |
| 34  | DM    | 24   | THR  | 3.5  |
| 45  | BY    | 22   | THR  | 3.5  |
| 27  | BE    | 115  | GLN  | 3.5  |
| 31  | BJ    | 86   | GLN  | 3.5  |
| 6   | AG    | 7    | GLY  | 3.5  |
| 7   | AH    | 121  | GLY  | 3.5  |
| 17  | CR    | 73   | HIS  | 3.5  |
| 25  | BC    | 52   | HIS  | 3.5  |
| 25  | BC    | 18   | VAL  | 3.5  |
| 26  | BD    | 20   | VAL  | 3.5  |
| 26  | DD    | 170  | VAL  | 3.5  |
| 27  | DE    | 58   | LYS  | 3.5  |
| 31  | BJ    | 39   | LYS  | 3.5  |
| 31  | BJ    | 63   | ALA  | 3.5  |
| 28  | DF    | 151  | LEU  | 3.5  |
| 26  | DD    | 88   | GLU  | 3.5  |
| 31  | DJ    | 95   | ARG  | 3.5  |
| 1   | AA    | 199  | A    | 3.5  |
| 1   | CA    | 1534 | A    | 3.5  |
| 23  | BB    | 144  | A    | 3.5  |
| 23  | DB    | 1275 | A    | 3.5  |
| 4   | AE    | 72   | ASN  | 3.5  |
| 15  | AP    | 79   | ASN  | 3.5  |
| 1   | AA    | 124  | C    | 3.5  |
| 21  | AU    | 36   | PHE  | 3.5  |
| 23  | BB    | 2310 | C    | 3.5  |
| 1   | AA    | 588  | G    | 3.5  |
| 25  | DC    | 5    | CYS  | 3.5  |
| 33  | DL    | 30   | THR  | 3.5  |
| 34  | BM    | 14   | LYS  | 3.5  |
| 13  | AN    | 3    | GLN  | 3.5  |
| 18  | CS    | 53   | GLY  | 3.5  |
| 26  | DD    | 92   | VAL  | 3.5  |
| 29  | BG    | 21   | GLN  | 3.5  |
| 36  | DO    | 91   | SER  | 3.5  |
| 41  | BT    | 15   | HIS  | 3.5  |
| 42  | DU    | 15   | GLY  | 3.5  |
| 43  | DW    | 30   | VAL  | 3.5  |
| 11  | CL    | 25   | ALA  | 3.5  |
| 15  | AP    | 82   | ALA  | 3.5  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 29  | BG    | 39   | ALA  | 3.5  |
| 39  | BR    | 28   | ALA  | 3.5  |
| 16  | AQ    | 7    | LEU  | 3.5  |
| 28  | BF    | 56   | LEU  | 3.5  |
| 1   | AA    | 1286 | U    | 3.5  |
| 8   | AI    | 45   | MET  | 3.5  |
| 45  | BY    | 41   | PRO  | 3.5  |
| 28  | DF    | 33   | ILE  | 3.5  |
| 4   | CE    | 92   | ARG  | 3.5  |
| 9   | CJ    | 47   | GLU  | 3.5  |
| 8   | CI    | 5    | TYR  | 3.5  |
| 3   | AD    | 19   | PHE  | 3.5  |
| 18  | AS    | 73   | PHE  | 3.5  |
| 27  | DE    | 98   | LYS  | 3.5  |
| 29  | DG    | 174  | LYS  | 3.5  |
| 31  | BJ    | 72   | LYS  | 3.5  |
| 38  | DQ    | 40   | LYS  | 3.5  |
| 25  | BC    | 222  | THR  | 3.5  |
| 25  | DC    | 219  | VAL  | 3.5  |
| 35  | BN    | 48   | VAL  | 3.5  |
| 43  | BW    | 30   | VAL  | 3.5  |
| 4   | CE    | 11   | GLN  | 3.5  |
| 29  | BG    | 63   | GLN  | 3.5  |
| 3   | AD    | 118  | SER  | 3.5  |
| 13  | AN    | 43   | ALA  | 3.5  |
| 17  | AR    | 66   | LEU  | 3.5  |
| 21  | CU    | 50   | SER  | 3.5  |
| 31  | DJ    | 109  | LEU  | 3.5  |
| 38  | DQ    | 59   | LEU  | 3.5  |
| 1   | AA    | 399  | G    | 3.5  |
| 1   | AA    | 633  | G    | 3.5  |
| 1   | CA    | 1002 | G    | 3.5  |
| 11  | AL    | 93   | ARG  | 3.5  |
| 12  | AM    | 112  | ARG  | 3.5  |
| 27  | BE    | 40   | ARG  | 3.5  |
| 28  | BF    | 149  | ARG  | 3.5  |
| 50  | B3    | 3    | ILE  | 3.5  |
| 23  | BB    | 1056 | G    | 3.5  |
| 23  | DB    | 1051 | G    | 3.5  |
| 29  | DG    | 43   | LYS  | 3.4  |
| 35  | DN    | 5    | LYS  | 3.4  |
| 48  | B1    | 24   | LYS  | 3.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 52  | BI    | 9    | LYS  | 3.4  |
| 18  | CS    | 73   | PHE  | 3.4  |
| 24  | BV    | 8    | VAL  | 3.4  |
| 37  | DP    | 65   | ASN  | 3.4  |
| 33  | DL    | 65   | GLY  | 3.4  |
| 35  | BN    | 79   | LEU  | 3.4  |
| 39  | BR    | 6    | GLN  | 3.4  |
| 40  | BS    | 10   | ALA  | 3.4  |
| 49  | D2    | 10   | LEU  | 3.4  |
| 2   | AC    | 175  | HIS  | 3.4  |
| 20  | CB    | 38   | HIS  | 3.4  |
| 28  | DF    | 4    | HIS  | 3.4  |
| 3   | AD    | 194  | ILE  | 3.4  |
| 3   | CD    | 2    | ARG  | 3.4  |
| 9   | AJ    | 76   | ILE  | 3.4  |
| 15  | AP    | 42   | ILE  | 3.4  |
| 16  | CQ    | 5    | ARG  | 3.4  |
| 18  | AS    | 29   | PRO  | 3.4  |
| 20  | CB    | 34   | ARG  | 3.4  |
| 25  | BC    | 226  | PRO  | 3.4  |
| 26  | BD    | 137  | SER  | 3.4  |
| 31  | DJ    | 113  | PRO  | 3.4  |
| 33  | DL    | 7    | SER  | 3.4  |
| 36  | DO    | 10   | ARG  | 3.4  |
| 42  | BU    | 5    | ARG  | 3.4  |
| 52  | BI    | 134  | SER  | 3.4  |
| 1   | AA    | 80   | A    | 3.4  |
| 23  | BB    | 1077 | A    | 3.4  |
| 23  | DB    | 899  | A    | 3.4  |
| 1   | AA    | 1214 | C    | 3.4  |
| 20  | AB    | 25   | LYS  | 3.4  |
| 23  | BB    | 11   | C    | 3.4  |
| 25  | BC    | 6    | LYS  | 3.4  |
| 41  | BT    | 36   | LYS  | 3.4  |
| 44  | BX    | 8    | GLU  | 3.4  |
| 35  | DN    | 102  | PHE  | 3.4  |
| 31  | DJ    | 74   | TYR  | 3.4  |
| 1   | AA    | 351  | G    | 3.4  |
| 11  | AL    | 118  | VAL  | 3.4  |
| 31  | BJ    | 62   | VAL  | 3.4  |
| 2   | AC    | 18   | ASN  | 3.4  |
| 4   | AE    | 27   | GLY  | 3.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 33  | DL    | 3    | LEU  | 3.4  |
| 35  | BN    | 107  | ASN  | 3.4  |
| 7   | CH    | 9    | MET  | 3.4  |
| 13  | CN    | 58   | ARG  | 3.4  |
| 16  | CQ    | 8    | GLN  | 3.4  |
| 35  | BN    | 91   | ALA  | 3.4  |
| 20  | AB    | 20   | ARG  | 3.4  |
| 20  | AB    | 135  | MET  | 3.4  |
| 40  | DS    | 1    | MET  | 3.4  |
| 43  | BW    | 29   | SER  | 3.4  |
| 25  | DC    | 206  | LYS  | 3.4  |
| 26  | DD    | 80   | TRP  | 3.4  |
| 37  | BP    | 62   | LYS  | 3.4  |
| 42  | DU    | 90   | LYS  | 3.4  |
| 27  | BE    | 145  | ASP  | 3.4  |
| 33  | BL    | 91   | ASP  | 3.4  |
| 26  | DD    | 99   | GLU  | 3.4  |
| 23  | DB    | 1057 | A    | 3.4  |
| 23  | DB    | 1098 | A    | 3.4  |
| 2   | CC    | 150  | VAL  | 3.4  |
| 17  | AR    | 39   | VAL  | 3.4  |
| 27  | BE    | 4    | VAL  | 3.4  |
| 41  | BT    | 61   | LEU  | 3.4  |
| 8   | CI    | 17   | ARG  | 3.4  |
| 13  | CN    | 52   | ARG  | 3.4  |
| 25  | DC    | 46   | GLY  | 3.4  |
| 31  | DJ    | 83   | GLY  | 3.4  |
| 20  | CB    | 11   | ALA  | 3.4  |
| 32  | BK    | 49   | ARG  | 3.4  |
| 32  | BK    | 119  | ALA  | 3.4  |
| 35  | BN    | 17   | ARG  | 3.4  |
| 43  | BW    | 83   | ALA  | 3.4  |
| 52  | BI    | 133  | ARG  | 3.4  |
| 52  | DI    | 26   | ALA  | 3.4  |
| 27  | BE    | 1    | MET  | 3.4  |
| 2   | AC    | 13   | ILE  | 3.4  |
| 6   | CG    | 6    | ILE  | 3.4  |
| 7   | CH    | 75   | GLN  | 3.4  |
| 23  | BB    | 2797 | U    | 3.4  |
| 35  | BN    | 13   | ASN  | 3.4  |
| 44  | BX    | 27   | ASN  | 3.4  |
| 9   | CJ    | 59   | LYS  | 3.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 13  | AN    | 46   | LYS  | 3.4  |
| 50  | D3    | 34   | LYS  | 3.4  |
| 1   | AA    | 462  | G    | 3.4  |
| 36  | BO    | 95   | SER  | 3.4  |
| 47  | D0    | 10   | SER  | 3.4  |
| 37  | DP    | 23   | ASP  | 3.4  |
| 5   | AF    | 39   | LEU  | 3.4  |
| 31  | BJ    | 125  | TYR  | 3.4  |
| 32  | BK    | 32   | TYR  | 3.4  |
| 39  | DR    | 2    | TYR  | 3.4  |
| 47  | D0    | 21   | LEU  | 3.4  |
| 52  | DI    | 52   | LEU  | 3.4  |
| 44  | BX    | 47   | ARG  | 3.4  |
| 18  | CS    | 43   | MET  | 3.4  |
| 27  | DE    | 199  | MET  | 3.4  |
| 34  | BM    | 82   | MET  | 3.4  |
| 23  | BB    | 2003 | A    | 3.4  |
| 23  | DB    | 878  | A    | 3.4  |
| 23  | DB    | 1913 | A    | 3.4  |
| 19  | AT    | 4    | LYS  | 3.4  |
| 24  | DV    | 87   | GLN  | 3.4  |
| 25  | DC    | 260  | LYS  | 3.4  |
| 27  | DE    | 57   | LYS  | 3.4  |
| 34  | DM    | 22   | GLN  | 3.4  |
| 38  | BQ    | 77   | LYS  | 3.4  |
| 47  | B0    | 40   | HIS  | 3.4  |
| 1   | AA    | 163  | C    | 3.4  |
| 1   | CA    | 422  | C    | 3.4  |
| 23  | BB    | 2666 | C    | 3.4  |
| 41  | DT    | 27   | SER  | 3.4  |
| 4   | CE    | 28   | ARG  | 3.4  |
| 6   | CG    | 104  | VAL  | 3.4  |
| 20  | AB    | 198  | VAL  | 3.4  |
| 21  | AU    | 28   | LEU  | 3.4  |
| 28  | BF    | 122  | ASP  | 3.4  |
| 39  | BR    | 26   | ASP  | 3.4  |
| 41  | DT    | 96   | VAL  | 3.4  |
| 51  | D4    | 36   | ARG  | 3.4  |
| 23  | DB    | 1524 | G    | 3.4  |
| 38  | BQ    | 75   | TYR  | 3.4  |
| 26  | DD    | 144  | GLY  | 3.4  |
| 27  | BE    | 26   | ALA  | 3.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 16  | AQ    | 15   | LYS  | 3.4  |
| 17  | AR    | 20   | ILE  | 3.4  |
| 27  | BE    | 77   | ILE  | 3.4  |
| 18  | AS    | 76   | THR  | 3.4  |
| 26  | DD    | 197  | THR  | 3.4  |
| 27  | BE    | 17   | THR  | 3.4  |
| 29  | BG    | 155  | PRO  | 3.4  |
| 34  | DM    | 98   | PRO  | 3.4  |
| 38  | DQ    | 13   | HIS  | 3.4  |
| 52  | BI    | 59   | THR  | 3.4  |
| 23  | BB    | 2058 | A    | 3.3  |
| 30  | DH    | 132  | PHE  | 3.3  |
| 31  | DJ    | 4    | PHE  | 3.3  |
| 1   | AA    | 183  | C    | 3.3  |
| 3   | AD    | 87   | GLU  | 3.3  |
| 7   | AH    | 71   | VAL  | 3.3  |
| 11  | AL    | 13   | ARG  | 3.3  |
| 12  | CM    | 55   | LEU  | 3.3  |
| 23  | BB    | 876  | C    | 3.3  |
| 24  | DV    | 38   | LEU  | 3.3  |
| 27  | BE    | 5    | LEU  | 3.3  |
| 33  | BL    | 69   | ARG  | 3.3  |
| 33  | BL    | 92   | LEU  | 3.3  |
| 38  | BQ    | 29   | ARG  | 3.3  |
| 12  | CM    | 109  | LYS  | 3.3  |
| 21  | AU    | 19   | LYS  | 3.3  |
| 25  | BC    | 46   | GLY  | 3.3  |
| 29  | DG    | 57   | TYR  | 3.3  |
| 35  | DN    | 125  | ALA  | 3.3  |
| 39  | BR    | 2    | TYR  | 3.3  |
| 49  | D2    | 38   | GLY  | 3.3  |
| 52  | DI    | 81   | LYS  | 3.3  |
| 37  | DP    | 109  | ILE  | 3.3  |
| 39  | DR    | 49   | ILE  | 3.3  |
| 34  | DM    | 60   | GLN  | 3.3  |
| 36  | DO    | 100  | HIS  | 3.3  |
| 45  | DY    | 33   | HIS  | 3.3  |
| 48  | D1    | 23   | THR  | 3.3  |
| 49  | D2    | 4    | THR  | 3.3  |
| 1   | AA    | 251  | G    | 3.3  |
| 34  | BM    | 28   | PHE  | 3.3  |
| 2   | AC    | 14   | VAL  | 3.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 20  | AB    | 134  | LEU  | 3.3  |
| 37  | BP    | 79   | VAL  | 3.3  |
| 37  | DP    | 46   | VAL  | 3.3  |
| 41  | DT    | 63   | VAL  | 3.3  |
| 1   | AA    | 353  | A    | 3.3  |
| 14  | AO    | 47   | LYS  | 3.3  |
| 23  | BB    | 1088 | A    | 3.3  |
| 23  | DB    | 1552 | A    | 3.3  |
| 27  | BE    | 80   | SER  | 3.3  |
| 33  | DL    | 141  | LYS  | 3.3  |
| 38  | DQ    | 92   | LYS  | 3.3  |
| 41  | DT    | 26   | LYS  | 3.3  |
| 11  | CL    | 1    | ALA  | 3.3  |
| 18  | CS    | 10   | ILE  | 3.3  |
| 26  | BD    | 93   | GLY  | 3.3  |
| 26  | BD    | 165  | MET  | 3.3  |
| 35  | DN    | 91   | ALA  | 3.3  |
| 36  | BO    | 44   | GLY  | 3.3  |
| 39  | DR    | 1    | MET  | 3.3  |
| 40  | DS    | 82   | MET  | 3.3  |
| 41  | BT    | 74   | ILE  | 3.3  |
| 47  | B0    | 1    | ALA  | 3.3  |
| 43  | BW    | 63   | ASP  | 3.3  |
| 48  | D1    | 20   | TYR  | 3.3  |
| 23  | DB    | 1458 | U    | 3.3  |
| 23  | BB    | 2385 | C    | 3.3  |
| 42  | BU    | 47   | PRO  | 3.3  |
| 13  | CN    | 66   | THR  | 3.3  |
| 25  | DC    | 251  | THR  | 3.3  |
| 42  | BU    | 76   | THR  | 3.3  |
| 45  | BY    | 29   | ARG  | 3.3  |
| 28  | DF    | 76   | PHE  | 3.3  |
| 33  | DL    | 64   | PHE  | 3.3  |
| 35  | DN    | 11   | ASN  | 3.3  |
| 45  | BY    | 16   | LEU  | 3.3  |
| 52  | BI    | 27   | LEU  | 3.3  |
| 52  | BI    | 97   | VAL  | 3.3  |
| 50  | D3    | 38   | LYS  | 3.3  |
| 1   | CA    | 1003 | G    | 3.3  |
| 2   | CC    | 153  | SER  | 3.3  |
| 4   | AE    | 109  | ALA  | 3.3  |
| 11  | AL    | 99   | GLY  | 3.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 15  | CP    | 43   | ALA  | 3.3  |
| 23  | BB    | 1510 | G    | 3.3  |
| 23  | BB    | 1813 | G    | 3.3  |
| 23  | DB    | 1235 | G    | 3.3  |
| 27  | DE    | 135  | ALA  | 3.3  |
| 30  | DH    | 65   | ALA  | 3.3  |
| 41  | BT    | 24   | MET  | 3.3  |
| 25  | DC    | 151  | GLY  | 3.3  |
| 39  | DR    | 50   | GLY  | 3.3  |
| 43  | DW    | 47   | GLY  | 3.3  |
| 20  | AB    | 21   | TYR  | 3.3  |
| 39  | DR    | 55   | ASP  | 3.3  |
| 22  | DA    | 25   | U    | 3.3  |
| 27  | BE    | 88   | ARG  | 3.3  |
| 35  | BN    | 4    | ARG  | 3.3  |
| 36  | BO    | 16   | ARG  | 3.3  |
| 39  | DR    | 6    | GLN  | 3.3  |
| 1   | AA    | 63   | C    | 3.3  |
| 9   | AJ    | 73   | LEU  | 3.3  |
| 24  | BV    | 91   | PHE  | 3.3  |
| 28  | DF    | 102  | LEU  | 3.3  |
| 6   | AG    | 113  | LYS  | 3.3  |
| 11  | CL    | 15   | VAL  | 3.3  |
| 30  | BH    | 21   | VAL  | 3.3  |
| 30  | BH    | 35   | LYS  | 3.3  |
| 33  | DL    | 1    | MET  | 3.3  |
| 20  | CB    | 165  | ALA  | 3.3  |
| 31  | BJ    | 134  | ALA  | 3.3  |
| 38  | BQ    | 26   | ALA  | 3.3  |
| 50  | B3    | 59   | ALA  | 3.3  |
| 52  | BI    | 85   | ILE  | 3.3  |
| 30  | BH    | 92   | GLY  | 3.3  |
| 26  | DD    | 139  | SER  | 3.3  |
| 36  | BO    | 45   | SER  | 3.3  |
| 52  | BI    | 87   | SER  | 3.3  |
| 14  | AO    | 63   | ARG  | 3.3  |
| 28  | DF    | 175  | PRO  | 3.3  |
| 31  | DJ    | 8    | PRO  | 3.3  |
| 35  | DN    | 90   | ARG  | 3.3  |
| 50  | B3    | 12   | ARG  | 3.3  |
| 52  | DI    | 22   | PRO  | 3.3  |
| 24  | DV    | 61   | LEU  | 3.3  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 27  | DE    | 12   | LEU  | 3.3  |
| 44  | BX    | 45   | GLN  | 3.3  |
| 52  | DI    | 10   | LEU  | 3.3  |
| 25  | BC    | 219  | VAL  | 3.3  |
| 34  | DM    | 108  | VAL  | 3.3  |
| 42  | BU    | 27   | VAL  | 3.3  |
| 23  | BB    | 1301 | A    | 3.3  |
| 23  | BB    | 1509 | A    | 3.3  |
| 23  | BB    | 1552 | A    | 3.3  |
| 3   | AD    | 36   | ALA  | 3.3  |
| 4   | CE    | 138  | ALA  | 3.3  |
| 19  | AT    | 66   | ILE  | 3.3  |
| 23  | BB    | 2103 | C    | 3.3  |
| 25  | BC    | 235  | GLU  | 3.3  |
| 27  | DE    | 190  | ALA  | 3.3  |
| 38  | BQ    | 98   | ALA  | 3.3  |
| 43  | BW    | 5    | ALA  | 3.3  |
| 14  | CO    | 15   | GLY  | 3.3  |
| 26  | BD    | 158  | GLY  | 3.3  |
| 29  | DG    | 56   | GLY  | 3.3  |
| 36  | DO    | 5    | SER  | 3.2  |
| 40  | BS    | 12   | SER  | 3.2  |
| 46  | DZ    | 15   | SER  | 3.2  |
| 25  | DC    | 187  | CYS  | 3.2  |
| 36  | DO    | 21   | LEU  | 3.2  |
| 16  | AQ    | 29   | LYS  | 3.2  |
| 19  | CT    | 74   | HIS  | 3.2  |
| 25  | BC    | 206  | LYS  | 3.2  |
| 32  | DK    | 67   | LYS  | 3.2  |
| 18  | CS    | 78   | THR  | 3.2  |
| 27  | BE    | 146  | VAL  | 3.2  |
| 28  | DF    | 24   | VAL  | 3.2  |
| 31  | DJ    | 11   | VAL  | 3.2  |
| 19  | AT    | 16   | ALA  | 3.2  |
| 27  | BE    | 175  | ILE  | 3.2  |
| 32  | DK    | 95   | ILE  | 3.2  |
| 43  | BW    | 35   | ILE  | 3.2  |
| 1   | AA    | 407  | U    | 3.2  |
| 16  | CQ    | 34   | GLY  | 3.2  |
| 20  | AB    | 32   | GLY  | 3.2  |
| 23  | BB    | 2139 | U    | 3.2  |
| 23  | BB    | 2801 | G    | 3.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 25  | DC    | 179  | GLU  | 3.2  |
| 23  | BB    | 2134 | A    | 3.2  |
| 27  | BE    | 44   | ARG  | 3.2  |
| 34  | DM    | 50   | ARG  | 3.2  |
| 2   | CC    | 50   | SER  | 3.2  |
| 23  | BB    | 1349 | C    | 3.2  |
| 12  | CM    | 95   | PRO  | 3.2  |
| 27  | DE    | 110  | SER  | 3.2  |
| 31  | BJ    | 121  | LYS  | 3.2  |
| 34  | DM    | 72   | PRO  | 3.2  |
| 34  | DM    | 78   | LEU  | 3.2  |
| 41  | DT    | 93   | LEU  | 3.2  |
| 44  | DX    | 40   | SER  | 3.2  |
| 50  | D3    | 4    | LYS  | 3.2  |
| 52  | BI    | 47   | SER  | 3.2  |
| 52  | BI    | 52   | LEU  | 3.2  |
| 19  | AT    | 30   | PHE  | 3.2  |
| 32  | BK    | 112  | PHE  | 3.2  |
| 30  | BH    | 142  | VAL  | 3.2  |
| 3   | AD    | 168  | THR  | 3.2  |
| 31  | DJ    | 93   | ILE  | 3.2  |
| 3   | AD    | 121  | ALA  | 3.2  |
| 4   | AE    | 124  | ALA  | 3.2  |
| 26  | DD    | 69   | ALA  | 3.2  |
| 7   | CH    | 122  | GLY  | 3.2  |
| 12  | AM    | 98   | GLY  | 3.2  |
| 14  | AO    | 88   | ARG  | 3.2  |
| 16  | AQ    | 64   | ARG  | 3.2  |
| 26  | BD    | 28   | GLU  | 3.2  |
| 27  | DE    | 51   | GLU  | 3.2  |
| 37  | BP    | 50   | ARG  | 3.2  |
| 31  | BJ    | 75   | TYR  | 3.2  |
| 1   | AA    | 219  | U    | 3.2  |
| 11  | CL    | 121  | PRO  | 3.2  |
| 42  | DU    | 47   | PRO  | 3.2  |
| 46  | DZ    | 7    | PRO  | 3.2  |
| 1   | AA    | 325  | A    | 3.2  |
| 3   | AD    | 129  | VAL  | 3.2  |
| 8   | CI    | 115  | VAL  | 3.2  |
| 20  | AB    | 15   | PHE  | 3.2  |
| 23  | BB    | 561  | G    | 3.2  |
| 23  | BB    | 831  | G    | 3.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 23  | BB    | 1475 | G    | 3.2  |
| 27  | BE    | 15   | SER  | 3.2  |
| 36  | DO    | 90   | VAL  | 3.2  |
| 37  | BP    | 18   | SER  | 3.2  |
| 42  | BU    | 24   | VAL  | 3.2  |
| 11  | AL    | 71   | HIS  | 3.2  |
| 20  | AB    | 14   | HIS  | 3.2  |
| 3   | CD    | 17   | ASP  | 3.2  |
| 23  | BB    | 2150 | C    | 3.2  |
| 23  | DB    | 11   | C    | 3.2  |
| 21  | AU    | 46   | ARG  | 3.2  |
| 33  | BL    | 97   | ALA  | 3.2  |
| 43  | DW    | 51   | GLY  | 3.2  |
| 34  | DM    | 127  | LYS  | 3.2  |
| 50  | D3    | 61   | LEU  | 3.2  |
| 36  | DO    | 99   | TYR  | 3.2  |
| 15  | AP    | 71   | VAL  | 3.2  |
| 18  | CS    | 60   | PHE  | 3.2  |
| 30  | BH    | 115  | VAL  | 3.2  |
| 37  | BP    | 60   | VAL  | 3.2  |
| 27  | BE    | 165  | HIS  | 3.2  |
| 47  | B0    | 4    | GLN  | 3.2  |
| 3   | AD    | 16   | THR  | 3.2  |
| 34  | DM    | 12   | MET  | 3.2  |
| 1   | AA    | 1014 | A    | 3.2  |
| 23  | BB    | 2108 | A    | 3.2  |
| 34  | DM    | 122  | ALA  | 3.2  |
| 1   | AA    | 724  | G    | 3.2  |
| 3   | AD    | 107  | GLY  | 3.2  |
| 4   | CE    | 13   | LYS  | 3.2  |
| 23  | BB    | 1738 | G    | 3.2  |
| 23  | DB    | 312  | G    | 3.2  |
| 23  | DB    | 1093 | G    | 3.2  |
| 23  | DB    | 2732 | G    | 3.2  |
| 25  | BC    | 25   | LYS  | 3.2  |
| 36  | BO    | 66   | GLY  | 3.2  |
| 39  | DR    | 73   | LYS  | 3.2  |
| 46  | BZ    | 2    | LYS  | 3.2  |
| 23  | BB    | 32   | C    | 3.2  |
| 23  | DB    | 143  | C    | 3.2  |
| 27  | DE    | 152  | GLU  | 3.2  |
| 28  | DF    | 90   | LEU  | 3.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 34  | BM    | 115  | GLU  | 3.2  |
| 36  | BO    | 80   | GLU  | 3.2  |
| 43  | BW    | 49   | ASN  | 3.2  |
| 17  | AR    | 50   | TYR  | 3.2  |
| 25  | BC    | 265  | PHE  | 3.2  |
| 34  | BM    | 4    | PRO  | 3.2  |
| 34  | BM    | 67   | VAL  | 3.2  |
| 43  | BW    | 59   | PHE  | 3.2  |
| 47  | B0    | 24   | VAL  | 3.2  |
| 12  | CM    | 78   | ARG  | 3.2  |
| 33  | BL    | 47   | ARG  | 3.2  |
| 43  | BW    | 40   | ARG  | 3.2  |
| 6   | CG    | 114  | SER  | 3.2  |
| 11  | AL    | 46   | SER  | 3.2  |
| 44  | DX    | 30   | MET  | 3.2  |
| 2   | AC    | 70   | ALA  | 3.2  |
| 8   | CI    | 42   | THR  | 3.2  |
| 27  | DE    | 87   | ALA  | 3.2  |
| 23  | BB    | 4    | U    | 3.1  |
| 23  | DB    | 102  | U    | 3.1  |
| 27  | DE    | 140  | ASP  | 3.1  |
| 27  | DE    | 145  | ASP  | 3.1  |
| 31  | DJ    | 26   | GLY  | 3.1  |
| 37  | DP    | 53   | GLY  | 3.1  |
| 52  | DI    | 98   | GLY  | 3.1  |
| 6   | AG    | 102  | TRP  | 3.1  |
| 25  | DC    | 153  | LEU  | 3.1  |
| 21  | AU    | 23   | GLU  | 3.1  |
| 37  | DP    | 43   | GLU  | 3.1  |
| 37  | DP    | 111  | GLU  | 3.1  |
| 39  | BR    | 16   | GLU  | 3.1  |
| 1   | AA    | 814  | A    | 3.1  |
| 23  | DB    | 391  | A    | 3.1  |
| 23  | DB    | 2297 | A    | 3.1  |
| 2   | AC    | 192  | TYR  | 3.1  |
| 29  | BG    | 42   | VAL  | 3.1  |
| 34  | DM    | 101  | VAL  | 3.1  |
| 43  | BW    | 22   | VAL  | 3.1  |
| 47  | D0    | 29   | VAL  | 3.1  |
| 33  | BL    | 119  | PRO  | 3.1  |
| 1   | AA    | 113  | G    | 3.1  |
| 1   | AA    | 328  | C    | 3.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 22  | BA    | 12   | C    | 3.1  |
| 22  | DA    | 118  | C    | 3.1  |
| 23  | BB    | 1311 | G    | 3.1  |
| 23  | BB    | 1980 | G    | 3.1  |
| 23  | BB    | 2138 | G    | 3.1  |
| 23  | BB    | 2780 | G    | 3.1  |
| 23  | DB    | 1    | G    | 3.1  |
| 23  | DB    | 1052 | C    | 3.1  |
| 23  | DB    | 1930 | G    | 3.1  |
| 23  | DB    | 2666 | C    | 3.1  |
| 9   | CJ    | 7    | ARG  | 3.1  |
| 13  | AN    | 40   | ARG  | 3.1  |
| 38  | BQ    | 52   | ARG  | 3.1  |
| 15  | AP    | 67   | ILE  | 3.1  |
| 40  | BS    | 74   | ILE  | 3.1  |
| 25  | DC    | 162  | GLN  | 3.1  |
| 38  | DQ    | 19   | GLN  | 3.1  |
| 8   | AI    | 119  | LYS  | 3.1  |
| 25  | DC    | 4    | LYS  | 3.1  |
| 14  | CO    | 24   | THR  | 3.1  |
| 25  | DC    | 60   | ALA  | 3.1  |
| 31  | BJ    | 41   | LYS  | 3.1  |
| 25  | DC    | 258  | SER  | 3.1  |
| 32  | BK    | 14   | SER  | 3.1  |
| 35  | BN    | 122  | ALA  | 3.1  |
| 4   | AE    | 141  | ASP  | 3.1  |
| 14  | AO    | 54   | GLY  | 3.1  |
| 25  | DC    | 26   | GLY  | 3.1  |
| 26  | BD    | 87   | GLY  | 3.1  |
| 38  | DQ    | 108  | LEU  | 3.1  |
| 25  | DC    | 34   | GLU  | 3.1  |
| 31  | DJ    | 9    | GLU  | 3.1  |
| 34  | BM    | 104  | GLU  | 3.1  |
| 34  | DM    | 104  | GLU  | 3.1  |
| 24  | BV    | 72   | VAL  | 3.1  |
| 34  | BM    | 130  | PHE  | 3.1  |
| 40  | BS    | 17   | VAL  | 3.1  |
| 52  | BI    | 60   | VAL  | 3.1  |
| 10  | CK    | 122  | PRO  | 3.1  |
| 25  | DC    | 202  | ARG  | 3.1  |
| 30  | BH    | 97   | ARG  | 3.1  |
| 31  | DJ    | 99   | ARG  | 3.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | CD    | 184  | LYS  | 3.1  |
| 12  | CM    | 52   | ILE  | 3.1  |
| 23  | BB    | 1757 | A    | 3.1  |
| 23  | DB    | 2108 | A    | 3.1  |
| 24  | DV    | 4    | ILE  | 3.1  |
| 26  | DD    | 157  | LYS  | 3.1  |
| 33  | BL    | 23   | ILE  | 3.1  |
| 41  | BT    | 30   | ILE  | 3.1  |
| 42  | BU    | 57   | ILE  | 3.1  |
| 39  | DR    | 89   | HIS  | 3.1  |
| 41  | BT    | 81   | LYS  | 3.1  |
| 45  | BY    | 20   | LYS  | 3.1  |
| 46  | DZ    | 70   | LYS  | 3.1  |
| 47  | B0    | 56   | LYS  | 3.1  |
| 51  | B4    | 2    | LYS  | 3.1  |
| 20  | CB    | 78   | ALA  | 3.1  |
| 27  | BE    | 41   | GLN  | 3.1  |
| 29  | DG    | 149  | ALA  | 3.1  |
| 39  | BR    | 42   | ALA  | 3.1  |
| 39  | DR    | 65   | ALA  | 3.1  |
| 41  | DT    | 99   | ALA  | 3.1  |
| 43  | BW    | 39   | GLN  | 3.1  |
| 1   | AA    | 83   | C    | 3.1  |
| 16  | AQ    | 43   | LEU  | 3.1  |
| 27  | DE    | 109  | LEU  | 3.1  |
| 34  | DM    | 128  | THR  | 3.1  |
| 41  | DT    | 8    | LEU  | 3.1  |
| 1   | AA    | 1039 | G    | 3.1  |
| 1   | CA    | 973  | G    | 3.1  |
| 13  | AN    | 67   | GLY  | 3.1  |
| 24  | DV    | 13   | GLY  | 3.1  |
| 32  | BK    | 34   | GLY  | 3.1  |
| 37  | DP    | 104  | GLY  | 3.1  |
| 31  | BJ    | 52   | ASP  | 3.1  |
| 4   | CE    | 135  | VAL  | 3.1  |
| 24  | DV    | 26   | PHE  | 3.1  |
| 38  | DQ    | 99   | VAL  | 3.1  |
| 38  | BQ    | 2    | ARG  | 3.1  |
| 43  | DW    | 59   | PHE  | 3.1  |
| 50  | D3    | 21   | PHE  | 3.1  |
| 50  | D3    | 39   | ARG  | 3.1  |
| 40  | BS    | 87   | PRO  | 3.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 50  | D3    | 45   | PRO  | 3.1  |
| 24  | BV    | 82   | TYR  | 3.1  |
| 20  | CB    | 39   | ILE  | 3.1  |
| 27  | DE    | 141  | MET  | 3.1  |
| 38  | DQ    | 21   | LYS  | 3.1  |
| 52  | BI    | 121  | ILE  | 3.1  |
| 12  | CM    | 105  | ALA  | 3.1  |
| 35  | BN    | 55   | ALA  | 3.1  |
| 36  | BO    | 50   | ALA  | 3.1  |
| 36  | DO    | 104  | GLN  | 3.1  |
| 51  | D4    | 29   | ALA  | 3.1  |
| 8   | CI    | 34   | LEU  | 3.1  |
| 27  | BE    | 105  | LEU  | 3.1  |
| 47  | D0    | 27   | LEU  | 3.1  |
| 1   | AA    | 51   | A    | 3.1  |
| 1   | AA    | 60   | A    | 3.1  |
| 1   | AA    | 1492 | A    | 3.1  |
| 1   | CA    | 65   | A    | 3.1  |
| 23  | BB    | 1237 | A    | 3.1  |
| 23  | DB    | 1596 | A    | 3.1  |
| 40  | BS    | 104  | THR  | 3.1  |
| 14  | AO    | 51   | SER  | 3.1  |
| 5   | CF    | 96   | VAL  | 3.1  |
| 6   | CG    | 66   | GLU  | 3.1  |
| 27  | BE    | 14   | VAL  | 3.1  |
| 30  | DH    | 37   | VAL  | 3.1  |
| 35  | BN    | 12   | ARG  | 3.1  |
| 41  | BT    | 67   | VAL  | 3.1  |
| 41  | DT    | 5    | GLU  | 3.1  |
| 44  | DX    | 24   | GLU  | 3.1  |
| 50  | D3    | 6    | VAL  | 3.1  |
| 51  | B4    | 12   | ARG  | 3.1  |
| 34  | BM    | 109  | PRO  | 3.1  |
| 46  | BZ    | 67   | PRO  | 3.1  |
| 22  | DA    | 24   | G    | 3.1  |
| 23  | BB    | 2133 | G    | 3.1  |
| 23  | DB    | 2110 | G    | 3.1  |
| 33  | BL    | 135  | ILE  | 3.1  |
| 39  | BR    | 101  | ILE  | 3.1  |
| 45  | BY    | 53   | MET  | 3.1  |
| 42  | BU    | 68   | ASN  | 3.1  |
| 6   | CG    | 38   | ALA  | 3.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 52  | BI    | 76   | ALA  | 3.1  |
| 1   | CA    | 1224 | U    | 3.1  |
| 12  | CM    | 79   | LEU  | 3.1  |
| 23  | BB    | 405  | U    | 3.1  |
| 23  | BB    | 2272 | U    | 3.1  |
| 27  | BE    | 3    | LEU  | 3.1  |
| 29  | DG    | 32   | LEU  | 3.1  |
| 52  | BI    | 137  | LEU  | 3.1  |
| 8   | AI    | 39   | GLY  | 3.1  |
| 9   | CJ    | 95   | GLY  | 3.1  |
| 39  | DR    | 8    | GLY  | 3.1  |
| 50  | D3    | 52   | GLY  | 3.1  |
| 19  | AT    | 59   | ARG  | 3.1  |
| 45  | BY    | 30   | ARG  | 3.1  |
| 27  | DE    | 96   | VAL  | 3.1  |
| 28  | DF    | 30   | VAL  | 3.1  |
| 39  | BR    | 72   | VAL  | 3.1  |
| 42  | DU    | 97   | SER  | 3.1  |
| 5   | CF    | 75   | GLU  | 3.1  |
| 15  | CP    | 32   | PHE  | 3.1  |
| 26  | BD    | 183  | GLU  | 3.1  |
| 28  | BF    | 13   | LYS  | 3.1  |
| 35  | DN    | 120  | GLU  | 3.1  |
| 37  | BP    | 42   | PHE  | 3.1  |
| 23  | BB    | 2872 | A    | 3.1  |
| 25  | DC    | 17   | LYS  | 3.1  |
| 42  | DU    | 16   | LYS  | 3.1  |
| 9   | AJ    | 75   | ASP  | 3.1  |
| 26  | BD    | 43   | ASP  | 3.1  |
| 29  | DG    | 38   | ASP  | 3.1  |
| 2   | AC    | 9    | ILE  | 3.1  |
| 34  | DM    | 1    | MET  | 3.1  |
| 37  | DP    | 4    | ILE  | 3.1  |
| 39  | BR    | 27   | ILE  | 3.1  |
| 42  | DU    | 57   | ILE  | 3.1  |
| 1   | AA    | 235  | C    | 3.0  |
| 23  | BB    | 982  | C    | 3.0  |
| 23  | BB    | 1072 | C    | 3.0  |
| 23  | DB    | 2143 | C    | 3.0  |
| 13  | CN    | 73   | LEU  | 3.0  |
| 17  | CR    | 67   | LEU  | 3.0  |
| 27  | DE    | 156  | ASN  | 3.0  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 35  | DN    | 25   | ALA  | 3.0  |
| 36  | BO    | 29   | HIS  | 3.0  |
| 28  | DF    | 134  | GLN  | 3.0  |
| 1   | CA    | 413  | G    | 3.0  |
| 23  | BB    | 726  | G    | 3.0  |
| 23  | DB    | 555  | G    | 3.0  |
| 23  | DB    | 1056 | G    | 3.0  |
| 23  | DB    | 1699 | G    | 3.0  |
| 25  | DC    | 13   | ARG  | 3.0  |
| 35  | BN    | 103  | ARG  | 3.0  |
| 47  | B0    | 49   | ARG  | 3.0  |
| 7   | AH    | 54   | THR  | 3.0  |
| 16  | AQ    | 69   | THR  | 3.0  |
| 29  | BG    | 35   | THR  | 3.0  |
| 1   | AA    | 472  | U    | 3.0  |
| 23  | BB    | 2689 | U    | 3.0  |
| 23  | DB    | 2903 | U    | 3.0  |
| 25  | DC    | 267  | VAL  | 3.0  |
| 29  | BG    | 167  | VAL  | 3.0  |
| 20  | AB    | 142  | LYS  | 3.0  |
| 26  | BD    | 90   | PHE  | 3.0  |
| 28  | DF    | 137  | PHE  | 3.0  |
| 29  | BG    | 108  | PHE  | 3.0  |
| 34  | BM    | 118  | LYS  | 3.0  |
| 36  | DO    | 56   | LYS  | 3.0  |
| 38  | DQ    | 15   | LYS  | 3.0  |
| 47  | D0    | 52   | LYS  | 3.0  |
| 49  | D2    | 25   | LYS  | 3.0  |
| 50  | D3    | 13   | PHE  | 3.0  |
| 2   | CC    | 21   | TRP  | 3.0  |
| 37  | DP    | 30   | TRP  | 3.0  |
| 51  | B4    | 6    | SER  | 3.0  |
| 4   | AE    | 110  | MET  | 3.0  |
| 4   | CE    | 83   | PRO  | 3.0  |
| 20  | CB    | 204  | ASP  | 3.0  |
| 27  | DE    | 116  | ASP  | 3.0  |
| 11  | AL    | 116  | TYR  | 3.0  |
| 8   | CI    | 117  | LEU  | 3.0  |
| 13  | AN    | 50   | LEU  | 3.0  |
| 19  | CT    | 46   | ALA  | 3.0  |
| 25  | BC    | 109  | LEU  | 3.0  |
| 23  | BB    | 1583 | A    | 3.0  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 26  | DD    | 31   | ALA  | 3.0  |
| 47  | D0    | 20   | ALA  | 3.0  |
| 20  | CB    | 14   | HIS  | 3.0  |
| 30  | DH    | 20   | ASN  | 3.0  |
| 1   | AA    | 106  | C    | 3.0  |
| 23  | BB    | 623  | C    | 3.0  |
| 9   | AJ    | 83   | THR  | 3.0  |
| 10  | AK    | 85   | VAL  | 3.0  |
| 29  | DG    | 16   | VAL  | 3.0  |
| 37  | BP    | 85   | VAL  | 3.0  |
| 40  | DS    | 83   | LYS  | 3.0  |
| 3   | AD    | 123  | MET  | 3.0  |
| 27  | DE    | 1    | MET  | 3.0  |
| 44  | BX    | 5    | GLU  | 3.0  |
| 8   | AI    | 29   | ILE  | 3.0  |
| 9   | AJ    | 100  | ILE  | 3.0  |
| 1   | AA    | 30   | U    | 3.0  |
| 1   | AA    | 471  | U    | 3.0  |
| 11  | AL    | 18   | SER  | 3.0  |
| 12  | CM    | 32   | ILE  | 3.0  |
| 13  | CN    | 57   | SER  | 3.0  |
| 18  | CS    | 3    | SER  | 3.0  |
| 30  | BH    | 143  | ILE  | 3.0  |
| 36  | DO    | 52   | SER  | 3.0  |
| 45  | BY    | 46   | MET  | 3.0  |
| 20  | AB    | 28   | PRO  | 3.0  |
| 23  | BB    | 102  | U    | 3.0  |
| 23  | BB    | 1082 | U    | 3.0  |
| 23  | DB    | 1101 | U    | 3.0  |
| 23  | DB    | 2180 | U    | 3.0  |
| 1   | CA    | 240  | G    | 3.0  |
| 23  | BB    | 914  | G    | 3.0  |
| 23  | BB    | 1653 | G    | 3.0  |
| 23  | BB    | 2405 | G    | 3.0  |
| 17  | AR    | 64   | LEU  | 3.0  |
| 19  | CT    | 65   | LEU  | 3.0  |
| 32  | BK    | 58   | LEU  | 3.0  |
| 39  | DR    | 25   | LEU  | 3.0  |
| 40  | DS    | 46   | LEU  | 3.0  |
| 5   | AF    | 49   | TYR  | 3.0  |
| 7   | CH    | 127  | TYR  | 3.0  |
| 13  | AN    | 35   | ALA  | 3.0  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 48  | B1    | 20   | TYR  | 3.0  |
| 48  | D1    | 1    | ALA  | 3.0  |
| 52  | DI    | 61   | TYR  | 3.0  |
| 42  | BU    | 93   | ARG  | 3.0  |
| 13  | CN    | 65   | GLN  | 3.0  |
| 15  | CP    | 46   | LYS  | 3.0  |
| 25  | BC    | 259  | ASN  | 3.0  |
| 27  | BE    | 94   | GLN  | 3.0  |
| 29  | BG    | 174  | LYS  | 3.0  |
| 44  | DX    | 38   | GLN  | 3.0  |
| 45  | DY    | 8    | GLN  | 3.0  |
| 1   | AA    | 1201 | A    | 3.0  |
| 23  | BB    | 1383 | A    | 3.0  |
| 23  | BB    | 1652 | A    | 3.0  |
| 28  | DF    | 73   | VAL  | 3.0  |
| 29  | DG    | 89   | VAL  | 3.0  |
| 33  | BL    | 5    | THR  | 3.0  |
| 1   | AA    | 1397 | C    | 3.0  |
| 8   | CI    | 64   | ILE  | 3.0  |
| 23  | BB    | 901  | C    | 3.0  |
| 26  | DD    | 48   | ILE  | 3.0  |
| 34  | DM    | 115  | GLU  | 3.0  |
| 37  | BP    | 70   | GLU  | 3.0  |
| 37  | BP    | 109  | ILE  | 3.0  |
| 46  | BZ    | 42   | PRO  | 3.0  |
| 50  | B3    | 45   | PRO  | 3.0  |
| 20  | AB    | 100  | LEU  | 3.0  |
| 27  | DE    | 179  | SER  | 3.0  |
| 39  | BR    | 25   | LEU  | 3.0  |
| 45  | DY    | 23   | LEU  | 3.0  |
| 4   | CE    | 16   | ALA  | 3.0  |
| 10  | AK    | 76   | TYR  | 3.0  |
| 14  | AO    | 57   | ARG  | 3.0  |
| 17  | AR    | 52   | ARG  | 3.0  |
| 24  | BV    | 18   | ARG  | 3.0  |
| 25  | DC    | 154  | ALA  | 3.0  |
| 27  | DE    | 50   | ALA  | 3.0  |
| 28  | BF    | 7    | TYR  | 3.0  |
| 29  | BG    | 163  | TYR  | 3.0  |
| 36  | DO    | 107  | ALA  | 3.0  |
| 40  | BS    | 89   | ALA  | 3.0  |
| 1   | AA    | 125  | U    | 3.0  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 23  | BB    | 12   | U    | 3.0  |
| 26  | DD    | 43   | ASP  | 3.0  |
| 33  | BL    | 14   | LYS  | 3.0  |
| 42  | BU    | 60   | LYS  | 3.0  |
| 45  | BY    | 55   | LYS  | 3.0  |
| 49  | B2    | 25   | LYS  | 3.0  |
| 2   | AC    | 194  | VAL  | 3.0  |
| 5   | CF    | 84   | VAL  | 3.0  |
| 10  | CK    | 120  | CYS  | 3.0  |
| 15  | CP    | 49   | GLY  | 3.0  |
| 26  | BD    | 66   | GLY  | 3.0  |
| 27  | DE    | 196  | VAL  | 3.0  |
| 28  | BF    | 30   | VAL  | 3.0  |
| 32  | BK    | 21   | CYS  | 3.0  |
| 34  | BM    | 45   | GLN  | 3.0  |
| 39  | DR    | 9    | GLY  | 3.0  |
| 23  | DB    | 1311 | G    | 3.0  |
| 23  | DB    | 1738 | G    | 3.0  |
| 52  | BI    | 69   | VAL  | 3.0  |
| 8   | CI    | 19   | PHE  | 3.0  |
| 12  | CM    | 107  | THR  | 3.0  |
| 4   | AE    | 133  | ILE  | 3.0  |
| 25  | BC    | 53   | ILE  | 3.0  |
| 38  | DQ    | 16   | ILE  | 3.0  |
| 52  | DI    | 135  | MET  | 3.0  |
| 8   | AI    | 51   | LEU  | 3.0  |
| 12  | CM    | 47   | LEU  | 3.0  |
| 19  | AT    | 65   | LEU  | 3.0  |
| 37  | BP    | 7    | LEU  | 3.0  |
| 42  | BU    | 36   | GLU  | 3.0  |
| 29  | DG    | 117  | PRO  | 3.0  |
| 34  | BM    | 69   | PRO  | 3.0  |
| 45  | DY    | 28   | LEU  | 3.0  |
| 32  | BK    | 18   | ARG  | 3.0  |
| 9   | CJ    | 54   | SER  | 3.0  |
| 1   | AA    | 110  | C    | 3.0  |
| 29  | BG    | 150  | TYR  | 3.0  |
| 31  | DJ    | 111  | LYS  | 3.0  |
| 33  | DL    | 109  | LYS  | 3.0  |
| 42  | DU    | 96   | LYS  | 3.0  |
| 44  | BX    | 2    | LYS  | 3.0  |
| 3   | AD    | 193  | ASP  | 3.0  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 10  | AK    | 77   | GLY  | 3.0  |
| 13  | AN    | 94   | GLY  | 3.0  |
| 19  | AT    | 41   | GLY  | 3.0  |
| 25  | BC    | 3    | VAL  | 3.0  |
| 25  | BC    | 14   | HIS  | 3.0  |
| 37  | BP    | 27   | VAL  | 3.0  |
| 37  | DP    | 85   | VAL  | 3.0  |
| 40  | BS    | 102  | HIS  | 3.0  |
| 42  | DU    | 33   | VAL  | 3.0  |
| 23  | DB    | 2320 | U    | 3.0  |
| 32  | BK    | 79   | PHE  | 3.0  |
| 35  | BN    | 87   | PHE  | 3.0  |
| 33  | BL    | 111  | ILE  | 3.0  |
| 16  | AQ    | 66   | LEU  | 2.9  |
| 39  | DR    | 22   | LEU  | 2.9  |
| 4   | AE    | 92   | ARG  | 2.9  |
| 1   | AA    | 105  | G    | 2.9  |
| 1   | AA    | 481  | G    | 2.9  |
| 11  | AL    | 10   | PRO  | 2.9  |
| 40  | BS    | 88   | ARG  | 2.9  |
| 40  | DS    | 18   | ARG  | 2.9  |
| 41  | BT    | 5    | GLU  | 2.9  |
| 23  | BB    | 2141 | G    | 2.9  |
| 3   | AD    | 148  | ALA  | 2.9  |
| 4   | CE    | 158  | LYS  | 2.9  |
| 38  | DQ    | 107  | ALA  | 2.9  |
| 41  | DT    | 19   | LYS  | 2.9  |
| 3   | CD    | 48   | SER  | 2.9  |
| 8   | CI    | 89   | TYR  | 2.9  |
| 16  | CQ    | 13   | SER  | 2.9  |
| 27  | BE    | 55   | SER  | 2.9  |
| 30  | DH    | 113  | SER  | 2.9  |
| 36  | BO    | 99   | TYR  | 2.9  |
| 37  | BP    | 77   | SER  | 2.9  |
| 47  | D0    | 47   | TYR  | 2.9  |
| 1   | CA    | 1285 | A    | 2.9  |
| 23  | BB    | 572  | A    | 2.9  |
| 23  | BB    | 1008 | A    | 2.9  |
| 23  | BB    | 1302 | A    | 2.9  |
| 23  | DB    | 2800 | A    | 2.9  |
| 12  | AM    | 63   | VAL  | 2.9  |
| 39  | DR    | 72   | VAL  | 2.9  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 43  | BW    | 55   | ASP  | 2.9  |
| 47  | B0    | 37   | HIS  | 2.9  |
| 27  | DE    | 124  | PHE  | 2.9  |
| 34  | DM    | 130  | PHE  | 2.9  |
| 1   | AA    | 488  | C    | 2.9  |
| 23  | DB    | 898  | C    | 2.9  |
| 20  | CB    | 150  | ILE  | 2.9  |
| 31  | DJ    | 1    | MET  | 2.9  |
| 38  | DQ    | 89   | ILE  | 2.9  |
| 52  | DI    | 85   | ILE  | 2.9  |
| 13  | CN    | 42   | ASN  | 2.9  |
| 15  | CP    | 6    | LEU  | 2.9  |
| 23  | DB    | 1340 | U    | 2.9  |
| 23  | DB    | 2182 | U    | 2.9  |
| 43  | BW    | 13   | ARG  | 2.9  |
| 2   | CC    | 200  | TRP  | 2.9  |
| 32  | DK    | 111  | LYS  | 2.9  |
| 36  | DO    | 55   | GLU  | 2.9  |
| 41  | BT    | 33   | LYS  | 2.9  |
| 43  | BW    | 16   | GLU  | 2.9  |
| 33  | BL    | 108  | ALA  | 2.9  |
| 45  | BY    | 21   | ALA  | 2.9  |
| 10  | CK    | 25   | SER  | 2.9  |
| 27  | BE    | 120  | VAL  | 2.9  |
| 33  | DL    | 68   | SER  | 2.9  |
| 52  | DI    | 97   | VAL  | 2.9  |
| 46  | DZ    | 29   | GLY  | 2.9  |
| 27  | DE    | 158  | PHE  | 2.9  |
| 3   | AD    | 28   | ASP  | 2.9  |
| 6   | AG    | 8    | GLN  | 2.9  |
| 9   | AJ    | 19   | ASP  | 2.9  |
| 16  | AQ    | 14   | ASP  | 2.9  |
| 29  | DG    | 46   | ASP  | 2.9  |
| 34  | BM    | 70   | ASP  | 2.9  |
| 26  | BD    | 48   | ILE  | 2.9  |
| 39  | DR    | 27   | ILE  | 2.9  |
| 52  | DI    | 34   | ILE  | 2.9  |
| 1   | AA    | 460  | A    | 2.9  |
| 1   | CA    | 415  | A    | 2.9  |
| 23  | DB    | 142  | A    | 2.9  |
| 23  | DB    | 1525 | A    | 2.9  |
| 25  | DC    | 23   | LEU  | 2.9  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 34  | BM    | 114 | ARG  | 2.9  |
| 34  | DM    | 112 | LEU  | 2.9  |
| 36  | BO    | 83  | LEU  | 2.9  |
| 38  | DQ    | 116 | LEU  | 2.9  |
| 42  | DU    | 93  | ARG  | 2.9  |
| 3   | AD    | 195 | ASN  | 2.9  |
| 6   | AG    | 34  | LYS  | 2.9  |
| 11  | AL    | 14  | LYS  | 2.9  |
| 20  | CB    | 35  | ASN  | 2.9  |
| 27  | DE    | 132 | LYS  | 2.9  |
| 28  | DF    | 13  | LYS  | 2.9  |
| 34  | DM    | 71  | LYS  | 2.9  |
| 12  | AM    | 114 | PRO  | 2.9  |
| 27  | BE    | 192 | ALA  | 2.9  |
| 28  | BF    | 57  | ALA  | 2.9  |
| 1   | CA    | 793 | U    | 2.9  |
| 23  | BB    | 50  | U    | 2.9  |
| 23  | BB    | 931 | U    | 2.9  |
| 6   | AG    | 79  | VAL  | 2.9  |
| 28  | BF    | 145 | VAL  | 2.9  |
| 2   | AC    | 154 | GLY  | 2.9  |
| 3   | CD    | 191 | SER  | 2.9  |
| 15  | AP    | 68  | SER  | 2.9  |
| 20  | CB    | 97  | GLY  | 2.9  |
| 24  | DV    | 15  | GLY  | 2.9  |
| 26  | DD    | 137 | SER  | 2.9  |
| 27  | DE    | 19  | PHE  | 2.9  |
| 27  | DE    | 183 | PHE  | 2.9  |
| 41  | BT    | 51  | PHE  | 2.9  |
| 46  | BZ    | 44  | PHE  | 2.9  |
| 49  | D2    | 8   | SER  | 2.9  |
| 18  | CS    | 68  | HIS  | 2.9  |
| 2   | AC    | 206 | ILE  | 2.9  |
| 9   | CJ    | 42  | LEU  | 2.9  |
| 15  | AP    | 6   | LEU  | 2.9  |
| 19  | CT    | 23  | ARG  | 2.9  |
| 27  | DE    | 175 | ILE  | 2.9  |
| 29  | BG    | 148 | ARG  | 2.9  |
| 32  | BK    | 17  | ARG  | 2.9  |
| 34  | BM    | 124 | LEU  | 2.9  |
| 35  | DN    | 98  | LEU  | 2.9  |
| 40  | BS    | 18  | ARG  | 2.9  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 41  | DT    | 61   | LEU  | 2.9  |
| 43  | BW    | 38   | ARG  | 2.9  |
| 52  | BI    | 135  | MET  | 2.9  |
| 27  | BE    | 176  | ASP  | 2.9  |
| 31  | DJ    | 19   | ASP  | 2.9  |
| 5   | CF    | 92   | THR  | 2.9  |
| 6   | AG    | 37   | THR  | 2.9  |
| 1   | AA    | 104  | G    | 2.9  |
| 1   | CA    | 86   | G    | 2.9  |
| 1   | CA    | 251  | G    | 2.9  |
| 2   | CC    | 24   | ASN  | 2.9  |
| 7   | CH    | 15   | ASN  | 2.9  |
| 30  | BH    | 96   | THR  | 2.9  |
| 40  | DS    | 3    | THR  | 2.9  |
| 37  | DP    | 101  | GLU  | 2.9  |
| 38  | DQ    | 114  | ALA  | 2.9  |
| 41  | DT    | 92   | ASN  | 2.9  |
| 45  | DY    | 9    | THR  | 2.9  |
| 12  | CM    | 71   | GLU  | 2.9  |
| 23  | BB    | 1115 | G    | 2.9  |
| 23  | BB    | 2458 | G    | 2.9  |
| 25  | BC    | 230  | PRO  | 2.9  |
| 30  | DH    | 111  | ALA  | 2.9  |
| 1   | AA    | 81   | A    | 2.9  |
| 1   | AA    | 143  | A    | 2.9  |
| 1   | AA    | 373  | A    | 2.9  |
| 1   | AA    | 1167 | A    | 2.9  |
| 23  | DB    | 1469 | A    | 2.9  |
| 8   | CI    | 54   | VAL  | 2.9  |
| 15  | CP    | 36   | VAL  | 2.9  |
| 27  | DE    | 121  | VAL  | 2.9  |
| 30  | BH    | 9    | VAL  | 2.9  |
| 1   | AA    | 54   | C    | 2.9  |
| 1   | AA    | 1281 | C    | 2.9  |
| 22  | BA    | 110  | C    | 2.9  |
| 23  | BB    | 1092 | C    | 2.9  |
| 23  | BB    | 1997 | C    | 2.9  |
| 23  | BB    | 2041 | U    | 2.9  |
| 25  | DC    | 61   | TYR  | 2.9  |
| 5   | AF    | 45   | ARG  | 2.9  |
| 10  | AK    | 60   | PHE  | 2.9  |
| 28  | DF    | 115  | GLY  | 2.9  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 43  | DW    | 10   | ARG  | 2.9  |
| 17  | AR    | 32   | ILE  | 2.9  |
| 24  | BV    | 61   | LEU  | 2.9  |
| 26  | DD    | 95   | SER  | 2.9  |
| 28  | BF    | 84   | ILE  | 2.9  |
| 28  | DF    | 117  | SER  | 2.9  |
| 29  | DG    | 36   | LEU  | 2.9  |
| 48  | B1    | 7    | LYS  | 2.9  |
| 26  | BD    | 108  | ASP  | 2.9  |
| 14  | AO    | 29   | ALA  | 2.9  |
| 15  | AP    | 11   | ALA  | 2.9  |
| 39  | BR    | 19   | THR  | 2.9  |
| 21  | AU    | 43   | GLU  | 2.9  |
| 26  | BD    | 89   | GLU  | 2.9  |
| 25  | BC    | 187  | CYS  | 2.9  |
| 18  | AS    | 9    | PHE  | 2.9  |
| 24  | DV    | 21   | ARG  | 2.9  |
| 25  | BC    | 237  | ARG  | 2.9  |
| 27  | DE    | 23   | PHE  | 2.9  |
| 27  | DE    | 174  | GLY  | 2.9  |
| 31  | DJ    | 37   | ARG  | 2.9  |
| 32  | BK    | 68   | GLY  | 2.9  |
| 33  | BL    | 59   | ARG  | 2.9  |
| 35  | DN    | 26   | GLY  | 2.9  |
| 36  | BO    | 96   | GLY  | 2.9  |
| 15  | CP    | 57   | ILE  | 2.9  |
| 23  | BB    | 101  | A    | 2.9  |
| 23  | BB    | 2062 | A    | 2.9  |
| 23  | BB    | 2682 | A    | 2.9  |
| 23  | DB    | 1236 | G    | 2.9  |
| 23  | DB    | 2503 | A    | 2.9  |
| 42  | BU    | 94   | PHE  | 2.9  |
| 48  | D1    | 48   | TYR  | 2.9  |
| 23  | DB    | 2844 | G    | 2.9  |
| 33  | BL    | 3    | LEU  | 2.9  |
| 36  | BO    | 17   | LYS  | 2.9  |
| 44  | DX    | 14   | LEU  | 2.9  |
| 45  | DY    | 53   | MET  | 2.9  |
| 51  | D4    | 18   | LYS  | 2.9  |
| 14  | CO    | 49   | HIS  | 2.8  |
| 1   | AA    | 1240 | U    | 2.8  |
| 1   | CA    | 421  | U    | 2.8  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | CA    | 1388 | C    | 2.8  |
| 23  | BB    | 1396 | U    | 2.8  |
| 23  | BB    | 2023 | C    | 2.8  |
| 23  | DB    | 1058 | U    | 2.8  |
| 23  | DB    | 1396 | U    | 2.8  |
| 23  | DB    | 2480 | C    | 2.8  |
| 24  | DV    | 75   | GLN  | 2.8  |
| 35  | BN    | 119  | SER  | 2.8  |
| 35  | DN    | 18   | GLN  | 2.8  |
| 38  | DQ    | 43   | GLN  | 2.8  |
| 18  | CS    | 11   | ASP  | 2.8  |
| 18  | CS    | 26   | ASP  | 2.8  |
| 2   | CC    | 173  | PRO  | 2.8  |
| 24  | DV    | 52   | ALA  | 2.8  |
| 25  | BC    | 243  | PRO  | 2.8  |
| 33  | DL    | 137  | ALA  | 2.8  |
| 14  | AO    | 25   | GLU  | 2.8  |
| 20  | CB    | 51   | GLU  | 2.8  |
| 37  | BP    | 101  | GLU  | 2.8  |
| 21  | CU    | 8    | ASN  | 2.8  |
| 27  | DE    | 113  | VAL  | 2.8  |
| 32  | BK    | 89   | ASN  | 2.8  |
| 39  | BR    | 51   | VAL  | 2.8  |
| 9   | AJ    | 7    | ARG  | 2.8  |
| 25  | BC    | 220  | ARG  | 2.8  |
| 33  | DL    | 21   | ARG  | 2.8  |
| 35  | BN    | 46   | ARG  | 2.8  |
| 43  | BW    | 76   | ARG  | 2.8  |
| 49  | D2    | 35   | ARG  | 2.8  |
| 24  | DV    | 2    | PHE  | 2.8  |
| 33  | DL    | 13   | LYS  | 2.8  |
| 33  | DL    | 129  | LYS  | 2.8  |
| 45  | DY    | 27   | GLY  | 2.8  |
| 50  | B3    | 11   | LYS  | 2.8  |
| 51  | B4    | 8    | LYS  | 2.8  |
| 2   | CC    | 167  | TYR  | 2.8  |
| 16  | AQ    | 24   | ILE  | 2.8  |
| 33  | BL    | 61   | LEU  | 2.8  |
| 37  | DP    | 113  | LEU  | 2.8  |
| 41  | BT    | 84   | TYR  | 2.8  |
| 12  | AM    | 13   | HIS  | 2.8  |
| 35  | DN    | 3    | HIS  | 2.8  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 46  | BZ    | 6    | HIS  | 2.8  |
| 1   | AA    | 356  | A    | 2.8  |
| 1   | AA    | 977  | A    | 2.8  |
| 8   | AI    | 92   | SER  | 2.8  |
| 42  | DU    | 53   | GLN  | 2.8  |
| 23  | DB    | 278  | A    | 2.8  |
| 26  | BD    | 54   | ALA  | 2.8  |
| 42  | DU    | 62   | ALA  | 2.8  |
| 44  | BX    | 3    | ALA  | 2.8  |
| 1   | AA    | 82   | G    | 2.8  |
| 21  | CU    | 10   | PRO  | 2.8  |
| 23  | BB    | 136  | G    | 2.8  |
| 23  | BB    | 653  | U    | 2.8  |
| 23  | BB    | 1976 | U    | 2.8  |
| 23  | BB    | 2286 | G    | 2.8  |
| 23  | BB    | 2848 | G    | 2.8  |
| 23  | DB    | 27   | G    | 2.8  |
| 23  | DB    | 1210 | G    | 2.8  |
| 23  | DB    | 2148 | G    | 2.8  |
| 20  | CB    | 126  | ASP  | 2.8  |
| 1   | AA    | 995  | C    | 2.8  |
| 9   | AJ    | 16   | ARG  | 2.8  |
| 9   | CJ    | 57   | VAL  | 2.8  |
| 20  | CB    | 209  | VAL  | 2.8  |
| 23  | DB    | 2104 | C    | 2.8  |
| 26  | DD    | 81   | GLU  | 2.8  |
| 38  | DQ    | 38   | VAL  | 2.8  |
| 45  | BY    | 44   | ARG  | 2.8  |
| 4   | AE    | 25   | LYS  | 2.8  |
| 8   | AI    | 30   | ASN  | 2.8  |
| 25  | DC    | 254  | LYS  | 2.8  |
| 41  | BT    | 28   | ASN  | 2.8  |
| 45  | BY    | 2    | LYS  | 2.8  |
| 46  | BZ    | 3    | LYS  | 2.8  |
| 46  | DZ    | 65   | ASN  | 2.8  |
| 27  | DE    | 133  | LEU  | 2.8  |
| 31  | BJ    | 55   | ILE  | 2.8  |
| 31  | DJ    | 81   | ILE  | 2.8  |
| 33  | BL    | 26   | GLY  | 2.8  |
| 34  | BM    | 41   | LEU  | 2.8  |
| 37  | BP    | 47   | ILE  | 2.8  |
| 38  | DQ    | 72   | GLY  | 2.8  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 52  | BI    | 54   | ILE  | 2.8  |
| 29  | BG    | 156  | TYR  | 2.8  |
| 14  | CO    | 41   | HIS  | 2.8  |
| 3   | CD    | 35   | GLN  | 2.8  |
| 3   | CD    | 135  | GLN  | 2.8  |
| 26  | DD    | 173  | GLN  | 2.8  |
| 12  | AM    | 31   | ALA  | 2.8  |
| 15  | CP    | 24   | SER  | 2.8  |
| 34  | DM    | 21   | ALA  | 2.8  |
| 40  | BS    | 32   | ALA  | 2.8  |
| 49  | D2    | 36   | ALA  | 2.8  |
| 3   | AD    | 45   | PRO  | 2.8  |
| 21  | CU    | 20   | ARG  | 2.8  |
| 26  | BD    | 46   | ARG  | 2.8  |
| 11  | AL    | 36   | VAL  | 2.8  |
| 11  | CL    | 42   | LYS  | 2.8  |
| 14  | AO    | 21   | THR  | 2.8  |
| 32  | BK    | 63   | VAL  | 2.8  |
| 41  | DT    | 55   | VAL  | 2.8  |
| 42  | BU    | 66   | VAL  | 2.8  |
| 31  | BJ    | 123  | LYS  | 2.8  |
| 31  | DJ    | 68   | LYS  | 2.8  |
| 32  | DK    | 73   | ASP  | 2.8  |
| 52  | BI    | 91   | LYS  | 2.8  |
| 23  | BB    | 2778 | A    | 2.8  |
| 1   | CA    | 531  | U    | 2.8  |
| 8   | AI    | 19   | PHE  | 2.8  |
| 4   | CE    | 118  | GLY  | 2.8  |
| 7   | AH    | 81   | GLY  | 2.8  |
| 10  | CK    | 109  | ILE  | 2.8  |
| 23  | BB    | 138  | U    | 2.8  |
| 23  | BB    | 1340 | U    | 2.8  |
| 23  | BB    | 2182 | U    | 2.8  |
| 23  | DB    | 2109 | U    | 2.8  |
| 28  | DF    | 116  | LEU  | 2.8  |
| 28  | BF    | 66   | ILE  | 2.8  |
| 46  | BZ    | 60   | PHE  | 2.8  |
| 13  | CN    | 67   | GLY  | 2.8  |
| 25  | BC    | 236  | GLY  | 2.8  |
| 29  | DG    | 160  | GLY  | 2.8  |
| 1   | AA    | 755  | G    | 2.8  |
| 23  | BB    | 830  | G    | 2.8  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 23  | BB    | 2021 | C    | 2.8  |
| 23  | BB    | 2573 | C    | 2.8  |
| 23  | BB    | 2869 | G    | 2.8  |
| 23  | DB    | 1499 | C    | 2.8  |
| 9   | AJ    | 56   | HIS  | 2.8  |
| 25  | BC    | 141  | HIS  | 2.8  |
| 27  | BE    | 86   | ALA  | 2.8  |
| 34  | BM    | 21   | ALA  | 2.8  |
| 36  | DO    | 98   | GLN  | 2.8  |
| 3   | CD    | 114  | ARG  | 2.8  |
| 15  | AP    | 8    | ARG  | 2.8  |
| 17  | CR    | 56   | ARG  | 2.8  |
| 35  | BN    | 22   | ARG  | 2.8  |
| 41  | BT    | 76   | ARG  | 2.8  |
| 42  | DU    | 5    | ARG  | 2.8  |
| 2   | AC    | 150  | VAL  | 2.8  |
| 5   | CF    | 93   | LYS  | 2.8  |
| 8   | AI    | 127  | SER  | 2.8  |
| 20  | AB    | 46   | VAL  | 2.8  |
| 27  | BE    | 132  | LYS  | 2.8  |
| 30  | DH    | 110  | VAL  | 2.8  |
| 52  | DI    | 8    | VAL  | 2.8  |
| 3   | CD    | 29   | THR  | 2.8  |
| 13  | CN    | 85   | GLU  | 2.8  |
| 32  | DK    | 42   | THR  | 2.8  |
| 36  | BO    | 115  | LEU  | 2.8  |
| 38  | BQ    | 82   | LEU  | 2.8  |
| 39  | BR    | 39   | LEU  | 2.8  |
| 39  | DR    | 29   | THR  | 2.8  |
| 50  | B3    | 5    | THR  | 2.8  |
| 6   | CG    | 102  | TRP  | 2.8  |
| 4   | AE    | 128  | GLY  | 2.8  |
| 25  | BC    | 233  | GLY  | 2.8  |
| 25  | DC    | 145  | MET  | 2.8  |
| 42  | BU    | 73   | ASN  | 2.8  |
| 23  | BB    | 878  | A    | 2.8  |
| 23  | BB    | 1032 | A    | 2.8  |
| 23  | BB    | 1939 | U    | 2.8  |
| 23  | BB    | 2311 | A    | 2.8  |
| 23  | DB    | 1097 | U    | 2.8  |
| 6   | CG    | 152  | HIS  | 2.8  |
| 18  | AS    | 51   | HIS  | 2.8  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 20  | AB    | 169  | HIS  | 2.8  |
| 47  | D0    | 37   | HIS  | 2.8  |
| 46  | BZ    | 37   | CYS  | 2.8  |
| 12  | CM    | 89   | ARG  | 2.8  |
| 1   | CA    | 18   | C    | 2.8  |
| 1   | CA    | 1317 | C    | 2.8  |
| 2   | CC    | 2    | GLN  | 2.8  |
| 7   | AH    | 17   | GLN  | 2.8  |
| 11  | CL    | 14   | LYS  | 2.8  |
| 13  | AN    | 11   | LYS  | 2.8  |
| 21  | CU    | 48   | LYS  | 2.8  |
| 23  | BB    | 2001 | C    | 2.8  |
| 26  | BD    | 173  | GLN  | 2.8  |
| 27  | DE    | 36   | ALA  | 2.8  |
| 36  | DO    | 51   | ALA  | 2.8  |
| 52  | BI    | 94   | LYS  | 2.8  |
| 1   | AA    | 111  | G    | 2.8  |
| 23  | BB    | 976  | G    | 2.8  |
| 23  | DB    | 2867 | G    | 2.8  |
| 52  | DI    | 138  | VAL  | 2.8  |
| 17  | CR    | 35   | SER  | 2.8  |
| 27  | BE    | 138  | LEU  | 2.8  |
| 32  | BK    | 8    | LEU  | 2.8  |
| 52  | BI    | 79   | LEU  | 2.8  |
| 12  | AM    | 101  | THR  | 2.8  |
| 25  | DC    | 99   | GLU  | 2.8  |
| 48  | B1    | 50   | GLU  | 2.8  |
| 30  | BH    | 91   | PHE  | 2.7  |
| 47  | B0    | 54   | ILE  | 2.8  |
| 52  | DI    | 58   | ILE  | 2.8  |
| 5   | AF    | 88   | MET  | 2.7  |
| 27  | BE    | 78   | TRP  | 2.7  |
| 10  | CK    | 17   | ASP  | 2.7  |
| 30  | DH    | 24   | GLY  | 2.7  |
| 31  | BJ    | 71   | ASP  | 2.7  |
| 34  | BM    | 25   | ASP  | 2.7  |
| 35  | BN    | 72   | ASP  | 2.7  |
| 36  | BO    | 2    | ASP  | 2.7  |
| 32  | DK    | 9    | ASN  | 2.7  |
| 46  | BZ    | 20   | ASN  | 2.7  |
| 48  | B1    | 25   | ASN  | 2.7  |
| 3   | CD    | 164  | ARG  | 2.7  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 11  | AL    | 11   | ARG  | 2.7  |
| 26  | DD    | 7    | LYS  | 2.7  |
| 26  | DD    | 62   | LYS  | 2.7  |
| 36  | BO    | 79   | ALA  | 2.7  |
| 37  | DP    | 106  | ALA  | 2.7  |
| 1   | CA    | 373  | A    | 2.7  |
| 23  | BB    | 2474 | U    | 2.7  |
| 26  | BD    | 104  | VAL  | 2.7  |
| 40  | BS    | 71   | VAL  | 2.7  |
| 44  | BX    | 50   | VAL  | 2.7  |
| 52  | DI    | 12   | VAL  | 2.7  |
| 7   | AH    | 58   | LEU  | 2.7  |
| 34  | DM    | 95   | LEU  | 2.7  |
| 1   | AA    | 345  | C    | 2.7  |
| 1   | AA    | 880  | C    | 2.7  |
| 12  | AM    | 16   | ILE  | 2.7  |
| 15  | CP    | 42   | ILE  | 2.7  |
| 11  | AL    | 39   | THR  | 2.7  |
| 14  | AO    | 24   | THR  | 2.7  |
| 14  | AO    | 58   | MET  | 2.7  |
| 20  | AB    | 29   | PHE  | 2.7  |
| 20  | CB    | 68   | PHE  | 2.7  |
| 20  | CB    | 139  | GLU  | 2.7  |
| 23  | BB    | 806  | C    | 2.7  |
| 23  | DB    | 1211 | C    | 2.7  |
| 24  | DV    | 69   | GLU  | 2.7  |
| 27  | DE    | 197  | GLU  | 2.7  |
| 33  | DL    | 115  | GLU  | 2.7  |
| 38  | DQ    | 35   | PHE  | 2.7  |
| 40  | BS    | 24   | ILE  | 2.7  |
| 41  | DT    | 89   | GLU  | 2.7  |
| 43  | BW    | 69   | GLU  | 2.7  |
| 43  | DW    | 8    | SER  | 2.7  |
| 20  | AB    | 95   | TRP  | 2.7  |
| 26  | DD    | 198  | GLY  | 2.7  |
| 29  | DG    | 61   | TRP  | 2.7  |
| 34  | BM    | 37   | GLY  | 2.7  |
| 1   | CA    | 1258 | G    | 2.7  |
| 23  | BB    | 1631 | G    | 2.7  |
| 28  | DF    | 45   | ASP  | 2.7  |
| 31  | DJ    | 116  | ARG  | 2.7  |
| 37  | BP    | 92   | ARG  | 2.7  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 39  | BR    | 21   | ARG  | 2.7  |
| 41  | BT    | 12   | ARG  | 2.7  |
| 10  | CK    | 118  | ASN  | 2.7  |
| 24  | BV    | 34   | LYS  | 2.7  |
| 51  | B4    | 9    | LYS  | 2.7  |
| 13  | CN    | 35   | ALA  | 2.7  |
| 26  | DD    | 75   | ALA  | 2.7  |
| 28  | BF    | 42   | ALA  | 2.7  |
| 8   | CI    | 28   | VAL  | 2.7  |
| 9   | AJ    | 74   | VAL  | 2.7  |
| 10  | AK    | 31   | VAL  | 2.7  |
| 15  | CP    | 19   | VAL  | 2.7  |
| 16  | AQ    | 82   | VAL  | 2.7  |
| 35  | BN    | 29   | VAL  | 2.7  |
| 7   | AH    | 10   | LEU  | 2.7  |
| 13  | AN    | 51   | PRO  | 2.7  |
| 21  | AU    | 40   | PRO  | 2.7  |
| 1   | AA    | 387  | U    | 2.7  |
| 1   | AA    | 1212 | U    | 2.7  |
| 1   | AA    | 1301 | U    | 2.7  |
| 1   | CA    | 1286 | U    | 2.7  |
| 2   | CC    | 36   | PHE  | 2.7  |
| 23  | BB    | 646  | U    | 2.7  |
| 23  | DB    | 2474 | U    | 2.7  |
| 39  | BR    | 35   | PHE  | 2.7  |
| 45  | BY    | 31   | ILE  | 2.7  |
| 52  | BI    | 49   | GLU  | 2.7  |
| 1   | AA    | 196  | A    | 2.7  |
| 1   | CA    | 1201 | A    | 2.7  |
| 1   | CA    | 1216 | A    | 2.7  |
| 1   | CA    | 1257 | A    | 2.7  |
| 3   | AD    | 175  | GLY  | 2.7  |
| 17  | AR    | 46   | THR  | 2.7  |
| 23  | BB    | 1347 | A    | 2.7  |
| 23  | BB    | 2377 | A    | 2.7  |
| 23  | BB    | 2886 | A    | 2.7  |
| 23  | DB    | 1630 | A    | 2.7  |
| 31  | BJ    | 115  | GLY  | 2.7  |
| 41  | BT    | 21   | SER  | 2.7  |
| 26  | DD    | 8    | LYS  | 2.7  |
| 26  | DD    | 70   | LYS  | 2.7  |
| 28  | BF    | 32   | LYS  | 2.7  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 41  | DT    | 36   | LYS  | 2.7  |
| 17  | CR    | 71   | ASP  | 2.7  |
| 20  | AB    | 122  | ASP  | 2.7  |
| 23  | DB    | 1092 | C    | 2.7  |
| 2   | CC    | 179  | ALA  | 2.7  |
| 12  | CM    | 34   | ALA  | 2.7  |
| 15  | CP    | 79   | ASN  | 2.7  |
| 25  | DC    | 141  | HIS  | 2.7  |
| 27  | BE    | 50   | ALA  | 2.7  |
| 30  | BH    | 84   | ALA  | 2.7  |
| 31  | BJ    | 59   | ALA  | 2.7  |
| 31  | DJ    | 77   | HIS  | 2.7  |
| 32  | BK    | 16   | ALA  | 2.7  |
| 50  | B3    | 9    | ALA  | 2.7  |
| 52  | BI    | 43   | ALA  | 2.7  |
| 7   | AH    | 128  | VAL  | 2.7  |
| 11  | AL    | 15   | VAL  | 2.7  |
| 27  | DE    | 178  | VAL  | 2.7  |
| 35  | BN    | 60   | VAL  | 2.7  |
| 36  | DO    | 54   | VAL  | 2.7  |
| 39  | DR    | 47   | VAL  | 2.7  |
| 31  | DJ    | 122  | LEU  | 2.7  |
| 44  | DX    | 21   | LEU  | 2.7  |
| 1   | AA    | 527  | G    | 2.7  |
| 1   | CA    | 331  | G    | 2.7  |
| 15  | CP    | 41   | PRO  | 2.7  |
| 23  | BB    | 733  | G    | 2.7  |
| 23  | BB    | 2157 | G    | 2.7  |
| 23  | DB    | 1475 | G    | 2.7  |
| 29  | DG    | 11   | PRO  | 2.7  |
| 36  | BO    | 98   | GLN  | 2.7  |
| 6   | CG    | 41   | ILE  | 2.7  |
| 12  | CM    | 62   | PHE  | 2.7  |
| 13  | CN    | 30   | ILE  | 2.7  |
| 18  | CS    | 40   | PHE  | 2.7  |
| 32  | BK    | 22   | ILE  | 2.7  |
| 43  | BW    | 25   | PHE  | 2.7  |
| 51  | D4    | 26   | ILE  | 2.7  |
| 25  | DC    | 131  | MET  | 2.7  |
| 7   | AH    | 119  | GLY  | 2.7  |
| 16  | CQ    | 25   | GLU  | 2.7  |
| 21  | CU    | 38   | GLU  | 2.7  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 32  | BK    | 45   | GLU  | 2.7  |
| 34  | BM    | 75   | GLU  | 2.7  |
| 8   | AI    | 118  | ARG  | 2.7  |
| 19  | AT    | 17   | ARG  | 2.7  |
| 26  | BD    | 141  | ARG  | 2.7  |
| 27  | BE    | 173  | THR  | 2.7  |
| 31  | BJ    | 13   | ARG  | 2.7  |
| 33  | DL    | 5    | THR  | 2.7  |
| 33  | DL    | 121  | THR  | 2.7  |
| 38  | DQ    | 49   | ARG  | 2.7  |
| 2   | AC    | 17   | TRP  | 2.7  |
| 13  | AN    | 96   | LYS  | 2.7  |
| 19  | CT    | 32   | LYS  | 2.7  |
| 24  | BV    | 83   | LYS  | 2.7  |
| 41  | BT    | 29   | THR  | 2.7  |
| 50  | B3    | 37   | THR  | 2.7  |
| 23  | BB    | 2605 | U    | 2.7  |
| 1   | AA    | 1447 | A    | 2.7  |
| 23  | BB    | 1420 | A    | 2.7  |
| 23  | BB    | 2267 | A    | 2.7  |
| 23  | DB    | 1496 | A    | 2.7  |
| 5   | AF    | 99   | ALA  | 2.7  |
| 25  | BC    | 210  | ALA  | 2.7  |
| 26  | BD    | 196  | ALA  | 2.7  |
| 39  | DR    | 3    | ALA  | 2.7  |
| 52  | DI    | 13   | ALA  | 2.7  |
| 6   | AG    | 5    | VAL  | 2.7  |
| 9   | CJ    | 96   | VAL  | 2.7  |
| 25  | BC    | 215  | VAL  | 2.7  |
| 26  | DD    | 5    | VAL  | 2.7  |
| 26  | DD    | 142  | VAL  | 2.7  |
| 33  | DL    | 93   | ASN  | 2.7  |
| 35  | DN    | 83   | LEU  | 2.7  |
| 39  | BR    | 20   | VAL  | 2.7  |
| 51  | B4    | 10   | LEU  | 2.7  |
| 1   | AA    | 518  | C    | 2.7  |
| 1   | CA    | 1226 | C    | 2.7  |
| 6   | CG    | 8    | GLN  | 2.7  |
| 25  | BC    | 31   | PRO  | 2.7  |
| 27  | DE    | 119  | ILE  | 2.7  |
| 39  | DR    | 74   | ILE  | 2.7  |
| 52  | BI    | 108  | ILE  | 2.7  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 52  | DI    | 19   | PRO  | 2.7  |
| 6   | CG    | 30   | MET  | 2.7  |
| 9   | CJ    | 13   | PHE  | 2.7  |
| 26  | BD    | 82   | PHE  | 2.7  |
| 37  | DP    | 58   | PHE  | 2.7  |
| 52  | BI    | 37   | PHE  | 2.7  |
| 3   | CD    | 153  | ARG  | 2.7  |
| 4   | AE    | 53   | ARG  | 2.7  |
| 2   | AC    | 146  | LYS  | 2.7  |
| 25  | DC    | 234  | GLY  | 2.7  |
| 28  | DF    | 163  | GLU  | 2.7  |
| 37  | DP    | 37   | LYS  | 2.7  |
| 38  | BQ    | 21   | LYS  | 2.7  |
| 39  | BR    | 57   | GLY  | 2.7  |
| 40  | DS    | 73   | LYS  | 2.7  |
| 47  | D0    | 6    | LYS  | 2.7  |
| 49  | B2    | 11   | LYS  | 2.7  |
| 52  | BI    | 129  | GLU  | 2.7  |
| 25  | DC    | 50   | THR  | 2.7  |
| 27  | DE    | 53   | THR  | 2.7  |
| 1   | AA    | 450  | G    | 2.7  |
| 23  | BB    | 2722 | G    | 2.7  |
| 6   | AG    | 82   | SER  | 2.7  |
| 45  | BY    | 51   | SER  | 2.7  |
| 47  | B0    | 33   | SER  | 2.7  |
| 8   | AI    | 66   | VAL  | 2.7  |
| 14  | AO    | 26   | VAL  | 2.7  |
| 23  | BB    | 2506 | U    | 2.7  |
| 23  | BB    | 2713 | U    | 2.7  |
| 31  | DJ    | 64   | VAL  | 2.7  |
| 36  | BO    | 54   | VAL  | 2.7  |
| 37  | BP    | 29   | VAL  | 2.7  |
| 42  | DU    | 10   | VAL  | 2.7  |
| 2   | AC    | 92   | ASP  | 2.7  |
| 3   | AD    | 17   | ASP  | 2.7  |
| 14  | AO    | 50   | HIS  | 2.7  |
| 29  | BG    | 59   | ASP  | 2.7  |
| 29  | BG    | 113  | ASP  | 2.7  |
| 33  | DL    | 81   | ASP  | 2.7  |
| 42  | DU    | 80   | ASP  | 2.7  |
| 25  | DC    | 43   | ASN  | 2.7  |
| 36  | DO    | 67   | ASN  | 2.7  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 48  | D1    | 25   | ASN  | 2.7  |
| 1   | AA    | 236  | A    | 2.6  |
| 9   | CJ    | 39   | PRO  | 2.6  |
| 11  | CL    | 81   | ILE  | 2.6  |
| 12  | CM    | 99   | GLN  | 2.6  |
| 23  | BB    | 91   | A    | 2.6  |
| 23  | BB    | 2297 | A    | 2.6  |
| 23  | DB    | 279  | A    | 2.6  |
| 28  | BF    | 153  | ILE  | 2.6  |
| 29  | BG    | 140  | ILE  | 2.6  |
| 30  | DH    | 38   | PRO  | 2.6  |
| 33  | BL    | 142  | ILE  | 2.6  |
| 36  | BO    | 87   | ILE  | 2.6  |
| 30  | BH    | 132  | PHE  | 2.6  |
| 34  | BM    | 136  | MET  | 2.6  |
| 51  | B4    | 35   | GLN  | 2.6  |
| 52  | DI    | 16   | MET  | 2.6  |
| 8   | CI    | 98   | ARG  | 2.6  |
| 33  | DL    | 60   | ARG  | 2.6  |
| 45  | BY    | 10   | ARG  | 2.6  |
| 49  | B2    | 3    | ARG  | 2.6  |
| 16  | CQ    | 29   | LYS  | 2.6  |
| 19  | AT    | 15   | LYS  | 2.6  |
| 29  | BG    | 176  | LYS  | 2.6  |
| 31  | BJ    | 2    | LYS  | 2.6  |
| 42  | DU    | 20   | LYS  | 2.6  |
| 49  | D2    | 2    | LYS  | 2.6  |
| 1   | AA    | 436  | C    | 2.6  |
| 1   | CA    | 470  | C    | 2.6  |
| 7   | CH    | 42   | GLU  | 2.6  |
| 8   | AI    | 69   | GLY  | 2.6  |
| 15  | CP    | 30   | GLY  | 2.6  |
| 26  | DD    | 66   | GLY  | 2.6  |
| 33  | DL    | 26   | GLY  | 2.6  |
| 33  | DL    | 102  | GLY  | 2.6  |
| 22  | BA    | 68   | C    | 2.6  |
| 23  | BB    | 1053 | C    | 2.6  |
| 23  | BB    | 1726 | C    | 2.6  |
| 45  | BY    | 57   | GLU  | 2.6  |
| 46  | DZ    | 10   | GLU  | 2.6  |
| 13  | CN    | 49   | THR  | 2.6  |
| 48  | B1    | 22   | THR  | 2.6  |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 52         | BI           | 117        | THR         | 2.6         |
| 3          | AD           | 81         | LEU         | 2.6         |
| 4          | AE           | 10         | LEU         | 2.6         |
| 6          | AG           | 90         | VAL         | 2.6         |
| 7          | CH           | 73         | SER         | 2.6         |
| 15         | CP           | 73         | ALA         | 2.6         |
| 17         | CR           | 66         | LEU         | 2.6         |
| 27         | DE           | 28         | VAL         | 2.6         |
| 27         | DE           | 146        | VAL         | 2.6         |
| 30         | BH           | 6          | LEU         | 2.6         |
| 48         | B1           | 51         | ALA         | 2.6         |
| 50         | B3           | 32         | LEU         | 2.6         |
| 1          | CA           | 1297       | G           | 2.6         |
| 3          | AD           | 49         | ASP         | 2.6         |
| 4          | CE           | 141        | ASP         | 2.6         |
| 6          | CG           | 11         | ILE         | 2.6         |
| 7          | AH           | 6          | ILE         | 2.6         |
| 7          | CH           | 112        | ASP         | 2.6         |
| 16         | CQ           | 14         | ASP         | 2.6         |
| 22         | DA           | 67         | G           | 2.6         |
| 22         | DA           | 85         | G           | 2.6         |
| 23         | BB           | 974        | G           | 2.6         |
| 26         | BD           | 18         | ASP         | 2.6         |
| 26         | DD           | 14         | ILE         | 2.6         |
| 28         | BF           | 135        | ILE         | 2.6         |
| 33         | DL           | 105        | ILE         | 2.6         |
| 5          | CF           | 91         | ARG         | 2.6         |
| 1          | AA           | 485        | U           | 2.6         |
| 15         | AP           | 13         | LYS         | 2.6         |
| 19         | AT           | 7          | LYS         | 2.6         |
| 28         | BF           | 28         | PRO         | 2.6         |
| 31         | DJ           | 97         | PRO         | 2.6         |
| 38         | DQ           | 5          | ARG         | 2.6         |
| 42         | BU           | 6          | ARG         | 2.6         |
| 42         | DU           | 26         | ASN         | 2.6         |
| 52         | BI           | 22         | PRO         | 2.6         |
| 52         | BI           | 35         | MET         | 2.6         |
| 22         | DA           | 89         | U           | 2.6         |
| 23         | BB           | 1065       | U           | 2.6         |
| 23         | DB           | 387        | U           | 2.6         |
| 2          | AC           | 73         | GLY         | 2.6         |
| 7          | AH           | 52         | GLY         | 2.6         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 25  | BC    | 240  | GLY  | 2.6  |
| 25  | DC    | 126  | GLY  | 2.6  |
| 27  | BE    | 56   | GLY  | 2.6  |
| 40  | BS    | 63   | GLY  | 2.6  |
| 1   | CA    | 792  | A    | 2.6  |
| 23  | BB    | 6    | A    | 2.6  |
| 23  | DB    | 2062 | A    | 2.6  |
| 30  | DH    | 149  | GLU  | 2.6  |
| 25  | DC    | 49   | THR  | 2.6  |
| 33  | BL    | 118  | THR  | 2.6  |
| 35  | BN    | 57   | THR  | 2.6  |
| 35  | BN    | 70   | THR  | 2.6  |
| 8   | AI    | 16   | ALA  | 2.6  |
| 12  | CM    | 60   | ALA  | 2.6  |
| 31  | BJ    | 117  | ALA  | 2.6  |
| 36  | DO    | 23   | ALA  | 2.6  |
| 36  | DO    | 83   | LEU  | 2.6  |
| 49  | B2    | 20   | ALA  | 2.6  |
| 52  | DI    | 78   | LEU  | 2.6  |
| 1   | AA    | 178  | C    | 2.6  |
| 1   | AA    | 1140 | C    | 2.6  |
| 23  | BB    | 2006 | C    | 2.6  |
| 36  | DO    | 95   | SER  | 2.6  |
| 2   | AC    | 201  | ILE  | 2.6  |
| 3   | AD    | 103  | ARG  | 2.6  |
| 26  | BD    | 13   | ARG  | 2.6  |
| 26  | BD    | 33   | ARG  | 2.6  |
| 34  | BM    | 5    | LYS  | 2.6  |
| 36  | BO    | 13   | ARG  | 2.6  |
| 37  | DP    | 3    | ILE  | 2.6  |
| 52  | DI    | 133  | ARG  | 2.6  |
| 5   | AF    | 62   | MET  | 2.6  |
| 15  | CP    | 38   | PHE  | 2.6  |
| 29  | DG    | 125  | PRO  | 2.6  |
| 34  | DM    | 125  | PRO  | 2.6  |
| 37  | DP    | 42   | PHE  | 2.6  |
| 3   | AD    | 135  | GLN  | 2.6  |
| 8   | AI    | 109  | GLN  | 2.6  |
| 9   | CJ    | 97   | ASP  | 2.6  |
| 13  | AN    | 59   | GLN  | 2.6  |
| 52  | BI    | 141  | ASP  | 2.6  |
| 35  | DN    | 81   | ASN  | 2.6  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | CD    | 77   | GLU  | 2.6  |
| 4   | AE    | 144  | GLU  | 2.6  |
| 7   | AH    | 59   | GLU  | 2.6  |
| 12  | CM    | 46   | GLU  | 2.6  |
| 23  | BB    | 162  | U    | 2.6  |
| 40  | BS    | 2    | GLU  | 2.6  |
| 1   | AA    | 597  | G    | 2.6  |
| 1   | CA    | 1034 | G    | 2.6  |
| 1   | CA    | 1312 | G    | 2.6  |
| 1   | CA    | 1316 | G    | 2.6  |
| 23  | BB    | 701  | G    | 2.6  |
| 23  | BB    | 2697 | G    | 2.6  |
| 23  | DB    | 1332 | G    | 2.6  |
| 10  | AK    | 112  | VAL  | 2.6  |
| 16  | CQ    | 11   | VAL  | 2.6  |
| 20  | AB    | 11   | ALA  | 2.6  |
| 29  | BG    | 118  | ALA  | 2.6  |
| 34  | DM    | 54   | THR  | 2.6  |
| 38  | BQ    | 87   | VAL  | 2.6  |
| 41  | DT    | 35   | ALA  | 2.6  |
| 42  | BU    | 74   | ALA  | 2.6  |
| 1   | AA    | 98   | A    | 2.6  |
| 1   | AA    | 974  | A    | 2.6  |
| 1   | CA    | 460  | A    | 2.6  |
| 14  | AO    | 16   | ARG  | 2.6  |
| 20  | AB    | 10   | LYS  | 2.6  |
| 23  | DB    | 126  | A    | 2.6  |
| 23  | DB    | 2327 | A    | 2.6  |
| 42  | BU    | 42   | LYS  | 2.6  |
| 46  | BZ    | 23   | LYS  | 2.6  |
| 46  | DZ    | 62   | LYS  | 2.6  |
| 51  | B4    | 36   | ARG  | 2.6  |
| 2   | AC    | 41   | TYR  | 2.6  |
| 3   | AD    | 48   | SER  | 2.6  |
| 9   | CJ    | 53   | ILE  | 2.6  |
| 20  | CB    | 225  | SER  | 2.6  |
| 36  | DO    | 87   | ILE  | 2.6  |
| 42  | BU    | 64   | ILE  | 2.6  |
| 40  | BS    | 7    | HIS  | 2.6  |
| 48  | D1    | 13   | SER  | 2.6  |
| 20  | AB    | 49   | PHE  | 2.6  |
| 37  | BP    | 19   | PHE  | 2.6  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 49  | B2    | 7    | PRO  | 2.6  |
| 2   | AC    | 99   | GLN  | 2.6  |
| 23  | BB    | 2362 | C    | 2.6  |
| 23  | DB    | 1072 | C    | 2.6  |
| 12  | CM    | 57   | ASP  | 2.6  |
| 20  | AB    | 152  | ASP  | 2.6  |
| 39  | BR    | 55   | ASP  | 2.6  |
| 30  | DH    | 13   | GLY  | 2.6  |
| 44  | DX    | 27   | ASN  | 2.6  |
| 48  | B1    | 17   | GLY  | 2.6  |
| 48  | D1    | 17   | GLY  | 2.6  |
| 52  | BI    | 33   | ASN  | 2.6  |
| 4   | AE    | 75   | LEU  | 2.6  |
| 26  | DD    | 40   | LEU  | 2.6  |
| 26  | DD    | 86   | GLU  | 2.6  |
| 27  | BE    | 198  | GLU  | 2.6  |
| 31  | BJ    | 140  | LEU  | 2.6  |
| 33  | BL    | 86   | GLU  | 2.6  |
| 41  | BT    | 4    | GLU  | 2.6  |
| 4   | AE    | 153  | ALA  | 2.6  |
| 8   | CI    | 16   | ALA  | 2.6  |
| 20  | AB    | 208  | ALA  | 2.6  |
| 25  | DC    | 223  | ALA  | 2.6  |
| 27  | DE    | 49   | ARG  | 2.6  |
| 28  | DF    | 67   | THR  | 2.6  |
| 35  | DN    | 41   | ALA  | 2.6  |
| 49  | D2    | 23   | ALA  | 2.6  |
| 1   | CA    | 1049 | U    | 2.6  |
| 9   | CJ    | 68   | ARG  | 2.6  |
| 13  | CN    | 22   | LYS  | 2.6  |
| 23  | BB    | 846  | U    | 2.6  |
| 23  | BB    | 932  | U    | 2.6  |
| 23  | DB    | 405  | U    | 2.6  |
| 23  | DB    | 546  | U    | 2.6  |
| 28  | DF    | 124  | ARG  | 2.6  |
| 31  | BJ    | 15   | TRP  | 2.6  |
| 33  | DL    | 70   | LYS  | 2.6  |
| 34  | BM    | 44   | ARG  | 2.6  |
| 36  | BO    | 88   | LYS  | 2.6  |
| 38  | DQ    | 102  | LYS  | 2.6  |
| 50  | B3    | 14   | LYS  | 2.6  |
| 9   | AJ    | 40   | ILE  | 2.6  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 15  | AP    | 75   | ILE  | 2.6  |
| 25  | DC    | 53   | ILE  | 2.6  |
| 39  | DR    | 59   | ILE  | 2.6  |
| 24  | BV    | 1    | MET  | 2.6  |
| 1   | AA    | 324  | G    | 2.6  |
| 1   | AA    | 326  | G    | 2.6  |
| 1   | CA    | 942  | G    | 2.6  |
| 1   | CA    | 1491 | G    | 2.6  |
| 4   | AE    | 99   | SER  | 2.6  |
| 23  | BB    | 2004 | G    | 2.6  |
| 23  | BB    | 2067 | G    | 2.6  |
| 23  | DB    | 388  | G    | 2.6  |
| 23  | DB    | 2553 | G    | 2.6  |
| 26  | BD    | 156  | PHE  | 2.6  |
| 41  | BT    | 17   | SER  | 2.6  |
| 1   | AA    | 329  | A    | 2.6  |
| 1   | AA    | 994  | A    | 2.6  |
| 23  | BB    | 574  | A    | 2.6  |
| 23  | BB    | 1073 | A    | 2.6  |
| 23  | BB    | 2873 | A    | 2.6  |
| 25  | DC    | 240  | GLY  | 2.6  |
| 28  | BF    | 125  | GLY  | 2.6  |
| 29  | DG    | 55   | ASP  | 2.6  |
| 7   | CH    | 82   | LEU  | 2.6  |
| 9   | AJ    | 10   | LEU  | 2.6  |
| 20  | CB    | 128  | LEU  | 2.6  |
| 31  | BJ    | 25   | LEU  | 2.6  |
| 44  | BX    | 56   | LEU  | 2.6  |
| 23  | BB    | 527  | C    | 2.6  |
| 23  | DB    | 915  | C    | 2.6  |
| 43  | DW    | 28   | GLU  | 2.6  |
| 8   | CI    | 15   | ALA  | 2.6  |
| 19  | AT    | 80   | ALA  | 2.6  |
| 25  | BC    | 19   | VAL  | 2.6  |
| 27  | DE    | 201  | ALA  | 2.6  |
| 28  | DF    | 1    | ALA  | 2.6  |
| 30  | DH    | 41   | LYS  | 2.6  |
| 35  | DN    | 64   | ARG  | 2.6  |
| 46  | DZ    | 51   | VAL  | 2.6  |
| 49  | D2    | 3    | ARG  | 2.6  |
| 51  | D4    | 32   | LYS  | 2.6  |
| 52  | BI    | 112  | LYS  | 2.6  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | AC    | 181  | ILE  | 2.5  |
| 3   | AD    | 27   | ILE  | 2.5  |
| 13  | AN    | 30   | ILE  | 2.5  |
| 34  | DM    | 136  | MET  | 2.5  |
| 39  | BR    | 1    | MET  | 2.5  |
| 44  | BX    | 1    | MET  | 2.5  |
| 3   | AD    | 71   | PHE  | 2.5  |
| 30  | DH    | 29   | PHE  | 2.5  |
| 33  | DL    | 66   | PHE  | 2.5  |
| 18  | AS    | 79   | TYR  | 2.5  |
| 23  | DB    | 2203 | U    | 2.5  |
| 25  | BC    | 160  | TYR  | 2.5  |
| 37  | DP    | 76   | HIS  | 2.5  |
| 9   | AJ    | 55   | PRO  | 2.5  |
| 32  | BK    | 120  | PRO  | 2.5  |
| 16  | CQ    | 67   | SER  | 2.5  |
| 39  | BR    | 7    | SER  | 2.5  |
| 50  | D3    | 50   | SER  | 2.5  |
| 2   | AC    | 157  | GLY  | 2.5  |
| 4   | CE    | 90   | GLY  | 2.5  |
| 13  | AN    | 77   | GLY  | 2.5  |
| 20  | AB    | 123  | GLY  | 2.5  |
| 32  | DK    | 15   | GLY  | 2.5  |
| 34  | BM    | 39   | GLY  | 2.5  |
| 3   | CD    | 190  | LEU  | 2.5  |
| 6   | CG    | 117  | LEU  | 2.5  |
| 47  | B0    | 27   | LEU  | 2.5  |
| 1   | AA    | 1379 | G    | 2.5  |
| 1   | CA    | 203  | G    | 2.5  |
| 1   | CA    | 1094 | G    | 2.5  |
| 2   | AC    | 26   | LYS  | 2.5  |
| 5   | AF    | 79   | ARG  | 2.5  |
| 6   | AG    | 75   | LYS  | 2.5  |
| 14  | CO    | 67   | ASP  | 2.5  |
| 19  | AT    | 83   | ASN  | 2.5  |
| 21  | CU    | 52   | VAL  | 2.5  |
| 23  | DB    | 956  | G    | 2.5  |
| 23  | DB    | 1250 | G    | 2.5  |
| 24  | DV    | 90   | ASP  | 2.5  |
| 28  | DF    | 87   | LYS  | 2.5  |
| 39  | DR    | 4    | VAL  | 2.5  |
| 42  | BU    | 80   | ASP  | 2.5  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | AA    | 532  | A    | 2.5  |
| 1   | AA    | 1446 | A    | 2.5  |
| 1   | CA    | 32   | A    | 2.5  |
| 1   | CA    | 459  | A    | 2.5  |
| 1   | CA    | 1319 | A    | 2.5  |
| 11  | CL    | 61   | GLU  | 2.5  |
| 23  | BB    | 877  | A    | 2.5  |
| 23  | BB    | 2814 | A    | 2.5  |
| 23  | DB    | 1046 | A    | 2.5  |
| 35  | BN    | 25   | ALA  | 2.5  |
| 35  | DN    | 66   | ALA  | 2.5  |
| 34  | BM    | 24   | THR  | 2.5  |
| 36  | BO    | 12   | THR  | 2.5  |
| 41  | BT    | 86   | THR  | 2.5  |
| 8   | AI    | 56   | MET  | 2.5  |
| 1   | AA    | 87   | C    | 2.5  |
| 1   | AA    | 576  | C    | 2.5  |
| 1   | CA    | 1322 | C    | 2.5  |
| 23  | BB    | 1646 | C    | 2.5  |
| 23  | DB    | 509  | C    | 2.5  |
| 23  | DB    | 542  | C    | 2.5  |
| 37  | DP    | 19   | PHE  | 2.5  |
| 13  | AN    | 70   | HIS  | 2.5  |
| 19  | AT    | 55   | PRO  | 2.5  |
| 46  | BZ    | 41   | HIS  | 2.5  |
| 1   | AA    | 103  | U    | 2.5  |
| 1   | AA    | 1125 | U    | 2.5  |
| 1   | CA    | 463  | U    | 2.5  |
| 3   | AD    | 15   | GLY  | 2.5  |
| 6   | AG    | 81   | GLY  | 2.5  |
| 7   | CH    | 120  | LEU  | 2.5  |
| 18  | AS    | 7    | GLY  | 2.5  |
| 23  | DB    | 2324 | U    | 2.5  |
| 25  | BC    | 98   | GLY  | 2.5  |
| 30  | BH    | 122  | LEU  | 2.5  |
| 33  | DL    | 44   | GLY  | 2.5  |
| 36  | DO    | 45   | SER  | 2.5  |
| 51  | D4    | 28   | SER  | 2.5  |
| 52  | DI    | 127  | SER  | 2.5  |
| 11  | AL    | 109  | ARG  | 2.5  |
| 25  | BC    | 58   | LYS  | 2.5  |
| 40  | DS    | 27   | LYS  | 2.5  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 26  | DD    | 203  | VAL  | 2.5  |
| 27  | BE    | 113  | VAL  | 2.5  |
| 27  | DE    | 126  | VAL  | 2.5  |
| 32  | DK    | 122  | VAL  | 2.5  |
| 48  | D1    | 46   | VAL  | 2.5  |
| 51  | D4    | 17   | VAL  | 2.5  |
| 2   | AC    | 45   | GLU  | 2.5  |
| 2   | CC    | 182  | ASP  | 2.5  |
| 11  | AL    | 16   | ALA  | 2.5  |
| 13  | AN    | 53   | ASP  | 2.5  |
| 14  | CO    | 19   | ASN  | 2.5  |
| 19  | CT    | 52   | GLU  | 2.5  |
| 25  | BC    | 223  | ALA  | 2.5  |
| 27  | DE    | 144  | GLU  | 2.5  |
| 28  | DF    | 69   | ALA  | 2.5  |
| 35  | DN    | 117  | ASP  | 2.5  |
| 36  | DO    | 20   | GLU  | 2.5  |
| 38  | BQ    | 9    | ALA  | 2.5  |
| 39  | BR    | 23   | GLU  | 2.5  |
| 40  | DS    | 59   | GLU  | 2.5  |
| 9   | AJ    | 25   | ILE  | 2.5  |
| 10  | CK    | 115  | ILE  | 2.5  |
| 12  | AM    | 3    | ILE  | 2.5  |
| 42  | BU    | 11   | ILE  | 2.5  |
| 42  | DU    | 11   | ILE  | 2.5  |
| 31  | BJ    | 70   | THR  | 2.5  |
| 9   | AJ    | 49   | PHE  | 2.5  |
| 24  | DV    | 91   | PHE  | 2.5  |
| 27  | BE    | 19   | PHE  | 2.5  |
| 1   | AA    | 197  | A    | 2.5  |
| 1   | AA    | 205  | A    | 2.5  |
| 1   | AA    | 349  | A    | 2.5  |
| 1   | AA    | 533  | A    | 2.5  |
| 23  | BB    | 1054 | A    | 2.5  |
| 1   | AA    | 650  | G    | 2.5  |
| 1   | AA    | 890  | G    | 2.5  |
| 1   | AA    | 1139 | G    | 2.5  |
| 22  | BA    | 100  | G    | 2.5  |
| 23  | BB    | 411  | G    | 2.5  |
| 23  | BB    | 1248 | G    | 2.5  |
| 23  | BB    | 2791 | G    | 2.5  |
| 23  | DB    | 1215 | G    | 2.5  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 11  | AL    | 95   | HIS  | 2.5  |
| 3   | AD    | 57   | LYS  | 2.5  |
| 3   | CD    | 7    | LYS  | 2.5  |
| 7   | AH    | 62   | LEU  | 2.5  |
| 9   | CJ    | 73   | LEU  | 2.5  |
| 8   | AI    | 68   | GLY  | 2.5  |
| 10  | AK    | 12   | ARG  | 2.5  |
| 13  | AN    | 8    | ARG  | 2.5  |
| 16  | CQ    | 3    | LYS  | 2.5  |
| 20  | CB    | 213  | LEU  | 2.5  |
| 25  | BC    | 173  | LEU  | 2.5  |
| 27  | BE    | 95   | LYS  | 2.5  |
| 27  | BE    | 117  | ARG  | 2.5  |
| 27  | BE    | 123  | LYS  | 2.5  |
| 27  | DE    | 118  | LEU  | 2.5  |
| 29  | BG    | 106  | LEU  | 2.5  |
| 23  | BB    | 2667 | C    | 2.5  |
| 23  | DB    | 2501 | C    | 2.5  |
| 29  | BG    | 157  | LYS  | 2.5  |
| 33  | BL    | 17   | LYS  | 2.5  |
| 40  | BS    | 91   | GLY  | 2.5  |
| 43  | BW    | 18   | LYS  | 2.5  |
| 50  | B3    | 34   | LYS  | 2.5  |
| 44  | BX    | 39   | GLN  | 2.5  |
| 51  | B4    | 11   | CYS  | 2.5  |
| 42  | DU    | 67   | SER  | 2.5  |
| 47  | D0    | 2    | VAL  | 2.5  |
| 30  | DH    | 26   | ALA  | 2.5  |
| 43  | BW    | 1    | ALA  | 2.5  |
| 43  | BW    | 32   | ALA  | 2.5  |
| 1   | AA    | 239  | U    | 2.5  |
| 23  | DB    | 1081 | U    | 2.5  |
| 23  | DB    | 1412 | U    | 2.5  |
| 23  | DB    | 1486 | U    | 2.5  |
| 27  | DE    | 2    | GLU  | 2.5  |
| 27  | DE    | 191  | ASP  | 2.5  |
| 30  | DH    | 73   | ASN  | 2.5  |
| 31  | BJ    | 14   | ASP  | 2.5  |
| 40  | DS    | 4    | ILE  | 2.5  |
| 45  | DY    | 47   | ILE  | 2.5  |
| 45  | DY    | 48   | ASN  | 2.5  |
| 2   | AC    | 133  | MET  | 2.5  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 20  | AB    | 153  | MET  | 2.5  |
| 18  | AS    | 47   | THR  | 2.5  |
| 26  | BD    | 35   | THR  | 2.5  |
| 47  | D0    | 22   | THR  | 2.5  |
| 3   | AD    | 167  | PRO  | 2.5  |
| 18  | AS    | 58   | PRO  | 2.5  |
| 26  | BD    | 143  | PRO  | 2.5  |
| 6   | AG    | 29   | LEU  | 2.5  |
| 6   | AG    | 117  | LEU  | 2.5  |
| 9   | AJ    | 46   | LYS  | 2.5  |
| 12  | CM    | 112  | ARG  | 2.5  |
| 28  | DF    | 21   | TYR  | 2.5  |
| 31  | DJ    | 130  | HIS  | 2.5  |
| 31  | DJ    | 140  | LEU  | 2.5  |
| 32  | BK    | 44   | LYS  | 2.5  |
| 34  | BM    | 66   | ARG  | 2.5  |
| 42  | BU    | 43   | LYS  | 2.5  |
| 50  | B3    | 2    | LYS  | 2.5  |
| 1   | AA    | 72   | A    | 2.5  |
| 1   | AA    | 389  | A    | 2.5  |
| 12  | CM    | 83   | GLY  | 2.5  |
| 23  | DB    | 1548 | A    | 2.5  |
| 27  | DE    | 71   | GLY  | 2.5  |
| 28  | BF    | 130  | GLY  | 2.5  |
| 33  | BL    | 43   | GLY  | 2.5  |
| 33  | DL    | 139  | GLY  | 2.5  |
| 48  | D1    | 15   | GLY  | 2.5  |
| 3   | CD    | 39   | GLN  | 2.5  |
| 13  | CN    | 3    | GLN  | 2.5  |
| 13  | CN    | 13   | VAL  | 2.5  |
| 18  | AS    | 50   | VAL  | 2.5  |
| 29  | DG    | 168  | VAL  | 2.5  |
| 52  | DI    | 110  | GLN  | 2.5  |
| 1   | AA    | 31   | G    | 2.5  |
| 1   | AA    | 538  | G    | 2.5  |
| 1   | CA    | 111  | G    | 2.5  |
| 10  | AK    | 44   | ALA  | 2.5  |
| 23  | BB    | 2509 | G    | 2.5  |
| 23  | BB    | 2844 | G    | 2.5  |
| 23  | DB    | 818  | G    | 2.5  |
| 23  | DB    | 2269 | G    | 2.5  |
| 23  | DB    | 2644 | G    | 2.5  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 29  | DG    | 122  | ALA  | 2.5  |
| 33  | BL    | 137  | ALA  | 2.5  |
| 35  | DN    | 89   | SER  | 2.5  |
| 20  | AB    | 66   | ILE  | 2.5  |
| 1   | AA    | 136  | C    | 2.5  |
| 1   | AA    | 503  | C    | 2.5  |
| 23  | DB    | 544  | C    | 2.5  |
| 23  | DB    | 2606 | C    | 2.5  |
| 25  | BC    | 184  | GLU  | 2.5  |
| 4   | CE    | 63   | MET  | 2.5  |
| 52  | DI    | 124  | MET  | 2.5  |
| 20  | AB    | 35   | ASN  | 2.5  |
| 25  | DC    | 228  | ASP  | 2.5  |
| 26  | DD    | 18   | ASP  | 2.5  |
| 26  | DD    | 200  | ASP  | 2.5  |
| 35  | BN    | 23   | ASN  | 2.5  |
| 39  | BR    | 43   | ASN  | 2.5  |
| 1   | AA    | 1017 | U    | 2.5  |
| 1   | AA    | 1049 | U    | 2.5  |
| 8   | CI    | 8    | THR  | 2.5  |
| 15  | AP    | 66   | THR  | 2.5  |
| 23  | BB    | 2149 | U    | 2.5  |
| 23  | BB    | 2554 | U    | 2.5  |
| 23  | DB    | 2181 | U    | 2.5  |
| 45  | DY    | 3    | THR  | 2.5  |
| 11  | AL    | 115  | LYS  | 2.5  |
| 13  | AN    | 27   | LYS  | 2.5  |
| 19  | CT    | 33   | LYS  | 2.5  |
| 21  | AU    | 45   | LYS  | 2.5  |
| 21  | CU    | 24   | LYS  | 2.5  |
| 3   | CD    | 10   | LEU  | 2.5  |
| 26  | DD    | 184  | ARG  | 2.5  |
| 29  | BG    | 132  | LEU  | 2.5  |
| 30  | DH    | 50   | ARG  | 2.5  |
| 31  | BJ    | 96   | ARG  | 2.5  |
| 25  | DC    | 230  | PRO  | 2.5  |
| 33  | DL    | 6    | LEU  | 2.5  |
| 28  | DF    | 75   | GLY  | 2.5  |
| 35  | DN    | 93   | GLY  | 2.5  |
| 9   | CJ    | 51   | VAL  | 2.5  |
| 26  | BD    | 189  | VAL  | 2.5  |
| 36  | DO    | 78   | VAL  | 2.5  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 42  | DU    | 24   | VAL  | 2.5  |
| 52  | BI    | 139  | VAL  | 2.5  |
| 27  | BE    | 90   | GLN  | 2.5  |
| 27  | DE    | 195  | GLN  | 2.5  |
| 6   | AG    | 133  | ALA  | 2.4  |
| 52  | BI    | 13   | ALA  | 2.4  |
| 16  | AQ    | 54   | ILE  | 2.4  |
| 24  | BV    | 4    | ILE  | 2.4  |
| 24  | BV    | 30   | ILE  | 2.4  |
| 30  | BH    | 94   | ILE  | 2.4  |
| 32  | BK    | 41   | ILE  | 2.4  |
| 34  | DM    | 27   | SER  | 2.4  |
| 34  | DM    | 126  | ILE  | 2.4  |
| 46  | BZ    | 18   | CYS  | 2.4  |
| 1   | CA    | 441  | A    | 2.4  |
| 1   | CA    | 1318 | A    | 2.4  |
| 2   | AC    | 165  | GLU  | 2.4  |
| 3   | AD    | 162  | GLU  | 2.4  |
| 8   | AI    | 111  | GLU  | 2.4  |
| 23  | BB    | 478  | A    | 2.4  |
| 23  | BB    | 1654 | A    | 2.4  |
| 23  | DB    | 2872 | A    | 2.4  |
| 27  | BE    | 100  | MET  | 2.4  |
| 27  | BE    | 197  | GLU  | 2.4  |
| 21  | AU    | 11   | PHE  | 2.4  |
| 39  | DR    | 35   | PHE  | 2.4  |
| 2   | AC    | 184  | ASN  | 2.4  |
| 3   | AD    | 46   | ARG  | 2.4  |
| 5   | CF    | 81   | ASN  | 2.4  |
| 10  | AK    | 126  | ARG  | 2.4  |
| 13  | AN    | 6    | LYS  | 2.4  |
| 14  | CO    | 17   | ASP  | 2.4  |
| 21  | AU    | 17   | ARG  | 2.4  |
| 24  | DV    | 18   | ARG  | 2.4  |
| 25  | BC    | 27   | LYS  | 2.4  |
| 25  | DC    | 196  | ASN  | 2.4  |
| 29  | DG    | 136  | ASP  | 2.4  |
| 29  | DG    | 152  | ARG  | 2.4  |
| 32  | BK    | 82   | ASN  | 2.4  |
| 32  | DK    | 17   | ARG  | 2.4  |
| 32  | DK    | 53   | LYS  | 2.4  |
| 39  | BR    | 95   | ASP  | 2.4  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 40  | BS    | 22   | ASP  | 2.4  |
| 42  | DU    | 18   | LYS  | 2.4  |
| 50  | B3    | 38   | LYS  | 2.4  |
| 1   | AA    | 41   | G    | 2.4  |
| 1   | AA    | 141  | G    | 2.4  |
| 1   | AA    | 376  | G    | 2.4  |
| 1   | AA    | 470  | C    | 2.4  |
| 1   | AA    | 990  | C    | 2.4  |
| 1   | AA    | 1322 | C    | 2.4  |
| 1   | AA    | 1432 | G    | 2.4  |
| 1   | AA    | 1529 | G    | 2.4  |
| 3   | AD    | 29   | THR  | 2.4  |
| 1   | CA    | 934  | C    | 2.4  |
| 3   | CD    | 8    | LEU  | 2.4  |
| 4   | AE    | 35   | LEU  | 2.4  |
| 4   | CE    | 10   | LEU  | 2.4  |
| 7   | CH    | 39   | LEU  | 2.4  |
| 9   | AJ    | 92   | LEU  | 2.4  |
| 14  | CO    | 2    | LEU  | 2.4  |
| 19  | CT    | 78   | LEU  | 2.4  |
| 23  | BB    | 45   | G    | 2.4  |
| 23  | BB    | 1685 | C    | 2.4  |
| 23  | BB    | 2318 | G    | 2.4  |
| 23  | DB    | 2250 | G    | 2.4  |
| 23  | DB    | 2307 | G    | 2.4  |
| 31  | DJ    | 21   | THR  | 2.4  |
| 31  | DJ    | 65   | THR  | 2.4  |
| 33  | BL    | 74   | THR  | 2.4  |
| 10  | AK    | 88   | PRO  | 2.4  |
| 34  | DM    | 4    | PRO  | 2.4  |
| 1   | AA    | 29   | U    | 2.4  |
| 1   | AA    | 561  | U    | 2.4  |
| 23  | DB    | 1249 | U    | 2.4  |
| 23  | DB    | 1576 | U    | 2.4  |
| 23  | DB    | 2384 | U    | 2.4  |
| 25  | DC    | 229  | HIS  | 2.4  |
| 11  | AL    | 3    | VAL  | 2.4  |
| 27  | DE    | 83   | VAL  | 2.4  |
| 28  | BF    | 24   | VAL  | 2.4  |
| 30  | BH    | 110  | VAL  | 2.4  |
| 30  | DH    | 3    | VAL  | 2.4  |
| 32  | BK    | 26   | GLY  | 2.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 38  | BQ    | 3    | VAL  | 2.4  |
| 40  | BS    | 45   | VAL  | 2.4  |
| 42  | BU    | 15   | GLY  | 2.4  |
| 43  | DW    | 66   | VAL  | 2.4  |
| 33  | DL    | 72   | ALA  | 2.4  |
| 38  | DQ    | 45   | ALA  | 2.4  |
| 8   | CI    | 27   | ILE  | 2.4  |
| 35  | DN    | 52   | ILE  | 2.4  |
| 38  | BQ    | 39   | ILE  | 2.4  |
| 4   | CE    | 21   | SER  | 2.4  |
| 7   | CH    | 88   | LYS  | 2.4  |
| 16  | CQ    | 36   | PHE  | 2.4  |
| 12  | CM    | 92   | ARG  | 2.4  |
| 17  | AR    | 23   | LYS  | 2.4  |
| 41  | DT    | 95   | PHE  | 2.4  |
| 42  | BU    | 96   | LYS  | 2.4  |
| 50  | B3    | 21   | PHE  | 2.4  |
| 17  | AR    | 62   | ARG  | 2.4  |
| 32  | DK    | 108  | ARG  | 2.4  |
| 20  | CB    | 156  | LEU  | 2.4  |
| 29  | DG    | 71   | LEU  | 2.4  |
| 42  | BU    | 13   | LEU  | 2.4  |
| 44  | DX    | 19   | LEU  | 2.4  |
| 8   | CI    | 3    | ASN  | 2.4  |
| 28  | BF    | 22   | ASN  | 2.4  |
| 30  | DH    | 28   | ASN  | 2.4  |
| 26  | BD    | 200  | ASP  | 2.4  |
| 31  | BJ    | 24   | THR  | 2.4  |
| 32  | BK    | 6    | THR  | 2.4  |
| 37  | BP    | 75   | THR  | 2.4  |
| 47  | B0    | 5    | ASN  | 2.4  |
| 1   | AA    | 109  | A    | 2.4  |
| 1   | AA    | 1093 | A    | 2.4  |
| 1   | AA    | 1333 | A    | 2.4  |
| 1   | AA    | 1534 | A    | 2.4  |
| 1   | CA    | 1446 | A    | 2.4  |
| 14  | CO    | 20   | ASP  | 2.4  |
| 10  | AK    | 122  | PRO  | 2.4  |
| 23  | DB    | 613  | A    | 2.4  |
| 23  | DB    | 654  | A    | 2.4  |
| 23  | DB    | 2336 | A    | 2.4  |
| 43  | BW    | 14   | ASP  | 2.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 26  | BD    | 63   | PRO  | 2.4  |
| 25  | BC    | 231  | HIS  | 2.4  |
| 35  | BN    | 76   | VAL  | 2.4  |
| 37  | DP    | 91   | VAL  | 2.4  |
| 43  | DW    | 56   | HIS  | 2.4  |
| 44  | DX    | 11   | VAL  | 2.4  |
| 50  | D3    | 19   | GLY  | 2.4  |
| 1   | AA    | 1249 | C    | 2.4  |
| 1   | CA    | 1210 | C    | 2.4  |
| 3   | CD    | 79   | ALA  | 2.4  |
| 5   | CF    | 95   | ALA  | 2.4  |
| 17  | CR    | 55   | ALA  | 2.4  |
| 23  | BB    | 509  | C    | 2.4  |
| 23  | BB    | 921  | C    | 2.4  |
| 23  | BB    | 1498 | C    | 2.4  |
| 23  | DB    | 96   | C    | 2.4  |
| 23  | DB    | 1732 | C    | 2.4  |
| 23  | DB    | 2146 | C    | 2.4  |
| 27  | BE    | 136  | GLN  | 2.4  |
| 28  | DF    | 78   | ILE  | 2.4  |
| 28  | DF    | 140  | ILE  | 2.4  |
| 28  | DF    | 155  | ILE  | 2.4  |
| 33  | DL    | 98   | ALA  | 2.4  |
| 42  | BU    | 102  | ILE  | 2.4  |
| 42  | DU    | 63   | ALA  | 2.4  |
| 43  | BW    | 48   | ALA  | 2.4  |
| 49  | D2    | 20   | ALA  | 2.4  |
| 1   | CA    | 377  | G    | 2.4  |
| 1   | CA    | 530  | G    | 2.4  |
| 1   | CA    | 1305 | G    | 2.4  |
| 3   | AD    | 70   | GLN  | 2.4  |
| 22  | DA    | 13   | G    | 2.4  |
| 23  | BB    | 1087 | G    | 2.4  |
| 23  | BB    | 1113 | U    | 2.4  |
| 23  | BB    | 1511 | G    | 2.4  |
| 23  | BB    | 1584 | U    | 2.4  |
| 23  | BB    | 1842 | G    | 2.4  |
| 23  | BB    | 2140 | G    | 2.4  |
| 23  | BB    | 2802 | G    | 2.4  |
| 23  | DB    | 277  | G    | 2.4  |
| 23  | DB    | 2458 | G    | 2.4  |
| 44  | BX    | 38   | GLN  | 2.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 45  | BY    | 8   | GLN  | 2.4  |
| 19  | CT    | 27  | MET  | 2.4  |
| 4   | AE    | 13  | LYS  | 2.4  |
| 6   | CG    | 34  | LYS  | 2.4  |
| 2   | AC    | 104 | GLU  | 2.4  |
| 9   | CJ    | 66  | GLU  | 2.4  |
| 11  | AL    | 120 | ARG  | 2.4  |
| 25  | BC    | 17  | LYS  | 2.4  |
| 26  | BD    | 208 | LYS  | 2.4  |
| 28  | BF    | 8   | LYS  | 2.4  |
| 28  | BF    | 144 | LYS  | 2.4  |
| 41  | DT    | 88  | LYS  | 2.4  |
| 46  | DZ    | 3   | LYS  | 2.4  |
| 21  | CU    | 23  | GLU  | 2.4  |
| 43  | DW    | 78  | PHE  | 2.4  |
| 50  | B3    | 7   | ARG  | 2.4  |
| 26  | BD    | 174 | SER  | 2.4  |
| 38  | BQ    | 74  | SER  | 2.4  |
| 26  | DD    | 100 | LEU  | 2.4  |
| 44  | BX    | 19  | LEU  | 2.4  |
| 46  | BZ    | 16  | CYS  | 2.4  |
| 51  | D4    | 11  | CYS  | 2.4  |
| 6   | AG    | 15  | PRO  | 2.4  |
| 9   | AJ    | 41  | PRO  | 2.4  |
| 25  | BC    | 69  | ASN  | 2.4  |
| 25  | DC    | 28  | PRO  | 2.4  |
| 9   | CJ    | 74  | VAL  | 2.4  |
| 25  | BC    | 136 | VAL  | 2.4  |
| 30  | BH    | 103 | VAL  | 2.4  |
| 37  | DP    | 25  | VAL  | 2.4  |
| 12  | AM    | 11  | HIS  | 2.4  |
| 26  | DD    | 135 | GLY  | 2.4  |
| 34  | BM    | 87  | GLY  | 2.4  |
| 38  | BQ    | 13  | HIS  | 2.4  |
| 41  | DT    | 15  | HIS  | 2.4  |
| 44  | BX    | 41  | HIS  | 2.4  |
| 44  | DX    | 41  | HIS  | 2.4  |
| 9   | CJ    | 34  | ALA  | 2.4  |
| 25  | DC    | 105 | ALA  | 2.4  |
| 30  | BH    | 111 | ALA  | 2.4  |
| 39  | DR    | 36  | ALA  | 2.4  |
| 52  | DI    | 103 | ALA  | 2.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | AA    | 510  | A    | 2.4  |
| 1   | CA    | 250  | A    | 2.4  |
| 23  | DB    | 783  | A    | 2.4  |
| 23  | DB    | 1009 | A    | 2.4  |
| 23  | DB    | 2388 | A    | 2.4  |
| 23  | DB    | 2721 | A    | 2.4  |
| 23  | DB    | 2820 | A    | 2.4  |
| 5   | CF    | 17   | GLN  | 2.4  |
| 9   | CJ    | 64   | GLN  | 2.4  |
| 14  | AO    | 64   | LYS  | 2.4  |
| 20  | AB    | 36   | LYS  | 2.4  |
| 27  | DE    | 67   | ARG  | 2.4  |
| 33  | DL    | 36   | LYS  | 2.4  |
| 33  | DL    | 132  | ARG  | 2.4  |
| 37  | DP    | 13   | LYS  | 2.4  |
| 38  | DQ    | 10   | ARG  | 2.4  |
| 41  | DT    | 76   | ARG  | 2.4  |
| 1   | AA    | 89   | U    | 2.4  |
| 1   | AA    | 312  | C    | 2.4  |
| 1   | AA    | 1403 | C    | 2.4  |
| 1   | CA    | 534  | U    | 2.4  |
| 3   | AD    | 67   | LEU  | 2.4  |
| 12  | CM    | 18   | LEU  | 2.4  |
| 14  | CO    | 55   | LEU  | 2.4  |
| 20  | CB    | 147  | LEU  | 2.4  |
| 23  | BB    | 991  | C    | 2.4  |
| 23  | BB    | 1585 | C    | 2.4  |
| 23  | BB    | 2339 | C    | 2.4  |
| 23  | DB    | 113  | U    | 2.4  |
| 23  | DB    | 2155 | U    | 2.4  |
| 23  | DB    | 2605 | U    | 2.4  |
| 26  | DD    | 183  | GLU  | 2.4  |
| 29  | DG    | 123  | GLU  | 2.4  |
| 3   | AD    | 22   | SER  | 2.4  |
| 3   | AD    | 204  | SER  | 2.4  |
| 13  | CN    | 31   | SER  | 2.4  |
| 47  | D0    | 26   | SER  | 2.4  |
| 1   | AA    | 211  | G    | 2.4  |
| 1   | AA    | 413  | G    | 2.4  |
| 1   | AA    | 1331 | G    | 2.4  |
| 1   | AA    | 1491 | G    | 2.4  |
| 23  | BB    | 978  | G    | 2.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 23  | BB    | 1120 | G    | 2.4  |
| 23  | BB    | 2524 | G    | 2.4  |
| 23  | DB    | 1410 | G    | 2.4  |
| 23  | DB    | 1980 | G    | 2.4  |
| 23  | DB    | 2290 | G    | 2.4  |
| 23  | DB    | 2633 | G    | 2.4  |
| 8   | AI    | 47   | VAL  | 2.4  |
| 16  | AQ    | 31   | PRO  | 2.4  |
| 21  | AU    | 52   | VAL  | 2.4  |
| 27  | DE    | 193  | VAL  | 2.4  |
| 32  | BK    | 65   | THR  | 2.4  |
| 37  | DP    | 17   | PRO  | 2.4  |
| 41  | DT    | 47   | VAL  | 2.4  |
| 48  | B1    | 46   | VAL  | 2.4  |
| 2   | CC    | 184  | ASN  | 2.4  |
| 15  | AP    | 29   | ASN  | 2.4  |
| 2   | CC    | 117  | ASP  | 2.4  |
| 14  | CO    | 50   | HIS  | 2.4  |
| 15  | AP    | 62   | GLY  | 2.4  |
| 37  | BP    | 53   | GLY  | 2.4  |
| 43  | BW    | 75   | ASN  | 2.4  |
| 43  | DW    | 72   | GLY  | 2.4  |
| 44  | BX    | 20   | ASN  | 2.4  |
| 32  | BK    | 29   | HIS  | 2.4  |
| 52  | DI    | 51   | GLY  | 2.4  |
| 6   | CG    | 60   | ALA  | 2.4  |
| 10  | CK    | 66   | ALA  | 2.4  |
| 13  | CN    | 1    | ALA  | 2.4  |
| 14  | CO    | 77   | TYR  | 2.4  |
| 17  | AR    | 69   | TYR  | 2.4  |
| 21  | AU    | 49   | ALA  | 2.4  |
| 37  | BP    | 63   | ILE  | 2.4  |
| 40  | BS    | 54   | ALA  | 2.4  |
| 52  | BI    | 114  | ALA  | 2.4  |
| 39  | BR    | 48   | LYS  | 2.4  |
| 50  | D3    | 40   | LYS  | 2.4  |
| 20  | AB    | 136  | ARG  | 2.4  |
| 36  | BO    | 33   | ARG  | 2.4  |
| 42  | DU    | 6    | ARG  | 2.4  |
| 46  | DZ    | 63   | ARG  | 2.4  |
| 26  | BD    | 49   | GLN  | 2.4  |
| 4   | AE    | 94   | PHE  | 2.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 5   | AF    | 78   | PHE  | 2.4  |
| 8   | AI    | 126  | PHE  | 2.4  |
| 20  | AB    | 68   | PHE  | 2.4  |
| 27  | BE    | 153  | LEU  | 2.4  |
| 1   | AA    | 32   | A    | 2.4  |
| 1   | AA    | 573  | A    | 2.4  |
| 21  | CU    | 7    | GLU  | 2.4  |
| 23  | BB    | 63   | A    | 2.4  |
| 23  | BB    | 207  | A    | 2.4  |
| 23  | DB    | 83   | A    | 2.4  |
| 23  | DB    | 125  | A    | 2.4  |
| 23  | DB    | 1253 | A    | 2.4  |
| 23  | DB    | 1419 | A    | 2.4  |
| 23  | DB    | 2860 | A    | 2.4  |
| 1   | AA    | 173  | U    | 2.4  |
| 1   | AA    | 1364 | U    | 2.4  |
| 1   | CA    | 961  | U    | 2.4  |
| 1   | CA    | 1202 | U    | 2.4  |
| 18  | AS    | 8    | PRO  | 2.4  |
| 23  | BB    | 2022 | U    | 2.4  |
| 23  | BB    | 2884 | U    | 2.4  |
| 23  | BB    | 2891 | U    | 2.4  |
| 29  | BG    | 7    | PRO  | 2.4  |
| 36  | DO    | 42   | PRO  | 2.4  |
| 41  | BT    | 16   | VAL  | 2.4  |
| 41  | BT    | 63   | VAL  | 2.4  |
| 41  | DT    | 34   | VAL  | 2.4  |
| 52  | DI    | 25   | PRO  | 2.4  |
| 1   | AA    | 1038 | C    | 2.3  |
| 7   | CH    | 25   | THR  | 2.3  |
| 23  | BB    | 1104 | C    | 2.3  |
| 27  | BE    | 189  | THR  | 2.3  |
| 2   | CC    | 126  | ARG  | 2.3  |
| 6   | AG    | 6    | ILE  | 2.3  |
| 7   | CH    | 23   | ALA  | 2.3  |
| 9   | AJ    | 94   | ALA  | 2.3  |
| 9   | CJ    | 46   | LYS  | 2.3  |
| 19  | CT    | 20   | ASN  | 2.3  |
| 31  | DJ    | 20   | ALA  | 2.3  |
| 39  | BR    | 10   | LYS  | 2.3  |
| 6   | AG    | 14   | ASP  | 2.3  |
| 7   | AH    | 53   | ASP  | 2.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 15  | CP    | 14   | ARG  | 2.3  |
| 18  | CS    | 77   | ARG  | 2.3  |
| 40  | DS    | 11   | ARG  | 2.3  |
| 41  | DT    | 12   | ARG  | 2.3  |
| 42  | BU    | 81   | ARG  | 2.3  |
| 45  | BY    | 42   | ALA  | 2.3  |
| 44  | BX    | 49   | ASP  | 2.3  |
| 47  | B0    | 47   | TYR  | 2.3  |
| 48  | D1    | 47   | ILE  | 2.3  |
| 34  | DM    | 106  | ASP  | 2.3  |
| 19  | CT    | 26   | MET  | 2.3  |
| 1   | AA    | 94   | G    | 2.3  |
| 1   | AA    | 369  | G    | 2.3  |
| 23  | BB    | 1063 | G    | 2.3  |
| 23  | BB    | 1091 | G    | 2.3  |
| 23  | BB    | 2156 | G    | 2.3  |
| 23  | BB    | 2645 | G    | 2.3  |
| 23  | BB    | 2763 | G    | 2.3  |
| 23  | DB    | 530  | G    | 2.3  |
| 23  | DB    | 548  | G    | 2.3  |
| 23  | DB    | 690  | G    | 2.3  |
| 3   | AD    | 106  | PHE  | 2.3  |
| 3   | CD    | 20   | LEU  | 2.3  |
| 8   | CI    | 102  | PHE  | 2.3  |
| 9   | CJ    | 49   | PHE  | 2.3  |
| 11  | AL    | 56   | LEU  | 2.3  |
| 20  | CB    | 88   | GLN  | 2.3  |
| 26  | DD    | 84   | LEU  | 2.3  |
| 28  | BF    | 121  | PHE  | 2.3  |
| 28  | DF    | 113  | PHE  | 2.3  |
| 45  | BY    | 26   | LEU  | 2.3  |
| 51  | D4    | 35   | GLN  | 2.3  |
| 52  | DI    | 11   | GLN  | 2.3  |
| 52  | DI    | 30   | GLN  | 2.3  |
| 3   | CD    | 171  | GLU  | 2.3  |
| 7   | CH    | 46   | GLU  | 2.3  |
| 43  | DW    | 16   | GLU  | 2.3  |
| 43  | DW    | 82   | GLU  | 2.3  |
| 2   | AC    | 152  | VAL  | 2.3  |
| 28  | DF    | 88   | VAL  | 2.3  |
| 33  | DL    | 122  | VAL  | 2.3  |
| 34  | BM    | 89   | VAL  | 2.3  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 18  | CS    | 41   | PRO  | 2.3  |
| 1   | AA    | 1239 | A    | 2.3  |
| 1   | AA    | 1357 | A    | 2.3  |
| 4   | AE    | 90   | GLY  | 2.3  |
| 4   | CE    | 25   | LYS  | 2.3  |
| 6   | CG    | 24   | LYS  | 2.3  |
| 12  | CM    | 66   | GLY  | 2.3  |
| 13  | AN    | 22   | LYS  | 2.3  |
| 2   | AC    | 49   | ALA  | 2.3  |
| 6   | AG    | 28   | ILE  | 2.3  |
| 12  | AM    | 72   | ILE  | 2.3  |
| 13  | AN    | 49   | THR  | 2.3  |
| 15  | AP    | 30   | GLY  | 2.3  |
| 15  | AP    | 80   | LYS  | 2.3  |
| 23  | BB    | 1103 | A    | 2.3  |
| 23  | BB    | 1307 | A    | 2.3  |
| 23  | BB    | 2266 | A    | 2.3  |
| 23  | DB    | 1808 | A    | 2.3  |
| 23  | DB    | 2386 | A    | 2.3  |
| 36  | BO    | 91   | SER  | 2.3  |
| 37  | BP    | 1    | SER  | 2.3  |
| 24  | DV    | 3    | THR  | 2.3  |
| 26  | BD    | 114  | LYS  | 2.3  |
| 35  | BN    | 56   | LYS  | 2.3  |
| 38  | BQ    | 14   | LYS  | 2.3  |
| 39  | DR    | 10   | LYS  | 2.3  |
| 18  | AS    | 48   | ILE  | 2.3  |
| 25  | DC    | 220  | ARG  | 2.3  |
| 28  | DF    | 135  | ILE  | 2.3  |
| 34  | DM    | 81   | ARG  | 2.3  |
| 37  | BP    | 88   | ARG  | 2.3  |
| 43  | DW    | 26   | GLY  | 2.3  |
| 50  | D3    | 41   | ARG  | 2.3  |
| 25  | DC    | 169  | ALA  | 2.3  |
| 30  | BH    | 23   | ALA  | 2.3  |
| 37  | BP    | 48   | ALA  | 2.3  |
| 37  | BP    | 57   | ALA  | 2.3  |
| 37  | BP    | 76   | HIS  | 2.3  |
| 1   | AA    | 982  | U    | 2.3  |
| 1   | AA    | 1183 | U    | 2.3  |
| 4   | AE    | 95   | MET  | 2.3  |
| 4   | CE    | 18   | ASN  | 2.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 7   | AH    | 85   | TYR  | 2.3  |
| 11  | AL    | 45   | ASN  | 2.3  |
| 23  | BB    | 2185 | U    | 2.3  |
| 23  | BB    | 2585 | U    | 2.3  |
| 23  | DB    | 2372 | U    | 2.3  |
| 25  | DC    | 170  | TYR  | 2.3  |
| 40  | BS    | 61   | ASN  | 2.3  |
| 1   | AA    | 526  | C    | 2.3  |
| 1   | AA    | 841  | C    | 2.3  |
| 1   | AA    | 862  | C    | 2.3  |
| 1   | AA    | 1344 | C    | 2.3  |
| 1   | CA    | 1533 | C    | 2.3  |
| 3   | AD    | 116  | LEU  | 2.3  |
| 5   | CF    | 54   | LEU  | 2.3  |
| 14  | AO    | 38   | LEU  | 2.3  |
| 23  | BB    | 2467 | C    | 2.3  |
| 23  | DB    | 1536 | C    | 2.3  |
| 27  | BE    | 191  | ASP  | 2.3  |
| 20  | AB    | 119  | GLN  | 2.3  |
| 25  | DC    | 265  | PHE  | 2.3  |
| 34  | DM    | 3    | GLN  | 2.3  |
| 34  | DM    | 31   | PHE  | 2.3  |
| 36  | BO    | 116  | GLN  | 2.3  |
| 37  | DP    | 14   | GLN  | 2.3  |
| 42  | BU    | 65   | GLN  | 2.3  |
| 52  | BI    | 5    | GLN  | 2.3  |
| 6   | AG    | 39   | GLU  | 2.3  |
| 16  | AQ    | 17   | GLU  | 2.3  |
| 20  | AB    | 117  | GLU  | 2.3  |
| 1   | AA    | 674  | G    | 2.3  |
| 1   | AA    | 1300 | G    | 2.3  |
| 1   | AA    | 1530 | G    | 2.3  |
| 1   | CA    | 462  | G    | 2.3  |
| 18  | CS    | 50   | VAL  | 2.3  |
| 23  | BB    | 1645 | G    | 2.3  |
| 23  | BB    | 2502 | G    | 2.3  |
| 23  | DB    | 450  | G    | 2.3  |
| 50  | B3    | 6    | VAL  | 2.3  |
| 52  | DI    | 23   | VAL  | 2.3  |
| 8   | CI    | 113  | LYS  | 2.3  |
| 13  | AN    | 97   | LYS  | 2.3  |
| 34  | DM    | 11   | LYS  | 2.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 41  | DT    | 49   | LYS  | 2.3  |
| 46  | DZ    | 39   | LYS  | 2.3  |
| 52  | BI    | 71   | LYS  | 2.3  |
| 52  | BI    | 96   | LYS  | 2.3  |
| 12  | CM    | 86   | ARG  | 2.3  |
| 21  | CU    | 16   | ARG  | 2.3  |
| 25  | DC    | 155  | ARG  | 2.3  |
| 26  | DD    | 205  | PRO  | 2.3  |
| 28  | DF    | 29   | ARG  | 2.3  |
| 31  | DJ    | 137  | PRO  | 2.3  |
| 34  | BM    | 38   | ARG  | 2.3  |
| 36  | DO    | 15   | ARG  | 2.3  |
| 43  | BW    | 10   | ARG  | 2.3  |
| 2   | AC    | 166  | TRP  | 2.3  |
| 4   | CE    | 31   | SER  | 2.3  |
| 12  | CM    | 21   | ILE  | 2.3  |
| 25  | DC    | 266  | ILE  | 2.3  |
| 26  | BD    | 144  | GLY  | 2.3  |
| 26  | DD    | 93   | GLY  | 2.3  |
| 27  | DE    | 151  | GLY  | 2.3  |
| 32  | DK    | 77   | ILE  | 2.3  |
| 39  | DR    | 30   | GLY  | 2.3  |
| 47  | B0    | 46   | GLY  | 2.3  |
| 16  | AQ    | 41   | THR  | 2.3  |
| 47  | B0    | 41   | HIS  | 2.3  |
| 52  | BI    | 16   | MET  | 2.3  |
| 38  | BQ    | 23   | TYR  | 2.3  |
| 51  | D4    | 14   | CYS  | 2.3  |
| 5   | AF    | 61   | LEU  | 2.3  |
| 6   | CG    | 29   | LEU  | 2.3  |
| 7   | AH    | 20   | ASN  | 2.3  |
| 10  | CK    | 99   | LEU  | 2.3  |
| 25  | BC    | 32   | LEU  | 2.3  |
| 27  | BE    | 112  | LEU  | 2.3  |
| 36  | DO    | 43   | ASN  | 2.3  |
| 1   | AA    | 412  | A    | 2.3  |
| 1   | AA    | 1216 | A    | 2.3  |
| 1   | CA    | 468  | A    | 2.3  |
| 1   | CA    | 983  | A    | 2.3  |
| 11  | AL    | 60   | PHE  | 2.3  |
| 22  | BA    | 29   | A    | 2.3  |
| 23  | BB    | 1084 | A    | 2.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 23  | BB    | 1095 | A    | 2.3  |
| 23  | BB    | 2037 | A    | 2.3  |
| 23  | DB    | 330  | A    | 2.3  |
| 23  | DB    | 2662 | A    | 2.3  |
| 26  | BD    | 176  | ASP  | 2.3  |
| 3   | AD    | 35   | GLN  | 2.3  |
| 23  | BB    | 2219 | U    | 2.3  |
| 23  | DB    | 2151 | U    | 2.3  |
| 37  | DP    | 40   | GLN  | 2.3  |
| 38  | BQ    | 19   | GLN  | 2.3  |
| 3   | AD    | 165  | GLU  | 2.3  |
| 20  | CB    | 144  | GLU  | 2.3  |
| 1   | AA    | 549  | C    | 2.3  |
| 1   | AA    | 1045 | C    | 2.3  |
| 1   | CA    | 1367 | C    | 2.3  |
| 2   | AC    | 79   | LYS  | 2.3  |
| 6   | CG    | 75   | LYS  | 2.3  |
| 8   | CI    | 18   | VAL  | 2.3  |
| 15  | AP    | 19   | VAL  | 2.3  |
| 23  | BB    | 184  | C    | 2.3  |
| 23  | BB    | 1639 | C    | 2.3  |
| 23  | BB    | 2755 | C    | 2.3  |
| 23  | DB    | 1114 | C    | 2.3  |
| 23  | DB    | 1595 | C    | 2.3  |
| 23  | DB    | 1606 | C    | 2.3  |
| 44  | BX    | 11   | VAL  | 2.3  |
| 49  | B2    | 9    | VAL  | 2.3  |
| 25  | DC    | 166  | ARG  | 2.3  |
| 37  | BP    | 20   | ARG  | 2.3  |
| 47  | D0    | 39   | ARG  | 2.3  |
| 7   | AH    | 13   | ILE  | 2.3  |
| 9   | CJ    | 67   | ILE  | 2.3  |
| 10  | CK    | 116  | PRO  | 2.3  |
| 18  | CS    | 48   | ILE  | 2.3  |
| 21  | AU    | 26   | GLY  | 2.3  |
| 26  | DD    | 96   | ILE  | 2.3  |
| 27  | DE    | 64   | GLY  | 2.3  |
| 28  | BF    | 92   | GLY  | 2.3  |
| 34  | BM    | 46   | ILE  | 2.3  |
| 34  | BM    | 96   | ILE  | 2.3  |
| 43  | BW    | 7    | GLY  | 2.3  |
| 29  | BG    | 12   | ALA  | 2.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 31  | BJ    | 20   | ALA  | 2.3  |
| 31  | DJ    | 6    | ALA  | 2.3  |
| 36  | BO    | 11   | ALA  | 2.3  |
| 38  | BQ    | 112  | ALA  | 2.3  |
| 40  | DS    | 89   | ALA  | 2.3  |
| 44  | DX    | 51   | ALA  | 2.3  |
| 2   | AC    | 128  | MET  | 2.3  |
| 5   | CF    | 87   | SER  | 2.3  |
| 12  | AM    | 19   | THR  | 2.3  |
| 14  | CO    | 3    | SER  | 2.3  |
| 26  | BD    | 16   | THR  | 2.3  |
| 27  | DE    | 125  | SER  | 2.3  |
| 39  | BR    | 102  | SER  | 2.3  |
| 47  | B0    | 26   | SER  | 2.3  |
| 52  | BI    | 20   | SER  | 2.3  |
| 38  | BQ    | 17   | LEU  | 2.3  |
| 38  | BQ    | 59   | LEU  | 2.3  |
| 1   | AA    | 881  | G    | 2.3  |
| 1   | AA    | 1386 | G    | 2.3  |
| 9   | CJ    | 65   | TYR  | 2.3  |
| 22  | DA    | 56   | G    | 2.3  |
| 22  | DA    | 100  | G    | 2.3  |
| 23  | BB    | 956  | G    | 2.3  |
| 23  | BB    | 1093 | G    | 2.3  |
| 23  | BB    | 1166 | G    | 2.3  |
| 23  | BB    | 2271 | G    | 2.3  |
| 23  | DB    | 124  | G    | 2.3  |
| 23  | DB    | 287  | G    | 2.3  |
| 23  | DB    | 2877 | G    | 2.3  |
| 36  | DO    | 36   | TYR  | 2.3  |
| 3   | AD    | 31   | CYS  | 2.3  |
| 31  | DJ    | 119  | PHE  | 2.3  |
| 37  | BP    | 114  | ASN  | 2.3  |
| 52  | BI    | 18   | ASN  | 2.3  |
| 3   | AD    | 189  | ASP  | 2.3  |
| 6   | CG    | 112  | ASP  | 2.3  |
| 9   | AJ    | 64   | GLN  | 2.3  |
| 20  | AB    | 126  | ASP  | 2.3  |
| 26  | BD    | 39   | ASP  | 2.3  |
| 29  | BG    | 55   | ASP  | 2.3  |
| 38  | BQ    | 51   | GLN  | 2.3  |
| 25  | BC    | 4    | LYS  | 2.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 38  | DQ    | 18   | LYS  | 2.3  |
| 1   | AA    | 1499 | A    | 2.3  |
| 1   | CA    | 452  | A    | 2.3  |
| 1   | CA    | 978  | A    | 2.3  |
| 4   | AE    | 20   | VAL  | 2.3  |
| 5   | AF    | 16   | GLU  | 2.3  |
| 13  | AN    | 58   | ARG  | 2.3  |
| 21  | CU    | 6    | ARG  | 2.3  |
| 23  | BB    | 613  | A    | 2.3  |
| 23  | BB    | 2800 | A    | 2.3  |
| 23  | DB    | 311  | A    | 2.3  |
| 23  | DB    | 2733 | A    | 2.3  |
| 26  | BD    | 99   | GLU  | 2.3  |
| 26  | BD    | 155  | VAL  | 2.3  |
| 26  | BD    | 168  | GLU  | 2.3  |
| 26  | DD    | 169  | ARG  | 2.3  |
| 27  | BE    | 193  | VAL  | 2.3  |
| 34  | BM    | 16   | ARG  | 2.3  |
| 40  | DS    | 20   | VAL  | 2.3  |
| 49  | B2    | 12   | ARG  | 2.3  |
| 49  | B2    | 39   | ARG  | 2.3  |
| 1   | AA    | 85   | U    | 2.3  |
| 1   | AA    | 180  | U    | 2.3  |
| 23  | DB    | 1061 | U    | 2.3  |
| 2   | AC    | 195  | ILE  | 2.3  |
| 33  | DL    | 135  | ILE  | 2.3  |
| 37  | DP    | 21   | PRO  | 2.3  |
| 10  | CK    | 91   | GLY  | 2.3  |
| 11  | CL    | 70   | GLY  | 2.3  |
| 27  | DE    | 142  | ALA  | 2.3  |
| 29  | BG    | 62   | ALA  | 2.3  |
| 31  | DJ    | 126  | ALA  | 2.3  |
| 33  | BL    | 15   | ALA  | 2.3  |
| 45  | DY    | 14   | GLY  | 2.3  |
| 52  | DI    | 136  | GLY  | 2.3  |
| 1   | AA    | 1001 | C    | 2.3  |
| 1   | CA    | 779  | C    | 2.3  |
| 23  | BB    | 145  | C    | 2.3  |
| 23  | BB    | 1607 | C    | 2.3  |
| 18  | CS    | 4    | LEU  | 2.3  |
| 25  | BC    | 245  | THR  | 2.3  |
| 30  | DH    | 96   | THR  | 2.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 46  | BZ    | 34   | LEU  | 2.3  |
| 31  | BJ    | 130  | HIS  | 2.3  |
| 31  | BJ    | 132  | HIS  | 2.3  |
| 48  | B1    | 16   | THR  | 2.3  |
| 52  | DI    | 111  | THR  | 2.3  |
| 20  | AB    | 31   | PHE  | 2.3  |
| 4   | AE    | 18   | ASN  | 2.3  |
| 5   | CF    | 52   | ASN  | 2.3  |
| 6   | CG    | 136  | LYS  | 2.3  |
| 12  | CM    | 77   | LYS  | 2.3  |
| 26  | DD    | 42   | ASN  | 2.3  |
| 31  | BJ    | 106  | LYS  | 2.3  |
| 45  | BY    | 48   | ASN  | 2.3  |
| 37  | DP    | 20   | ARG  | 2.3  |
| 40  | BS    | 15   | GLN  | 2.3  |
| 46  | DZ    | 37   | CYS  | 2.3  |
| 13  | AN    | 68   | ARG  | 2.3  |
| 20  | CB    | 20   | ARG  | 2.3  |
| 27  | BE    | 21   | ARG  | 2.3  |
| 31  | BJ    | 95   | ARG  | 2.3  |
| 3   | CD    | 128  | VAL  | 2.3  |
| 9   | AJ    | 60   | ASP  | 2.3  |
| 13  | AN    | 32   | ASP  | 2.3  |
| 25  | BC    | 164  | VAL  | 2.3  |
| 25  | BC    | 194  | VAL  | 2.3  |
| 26  | DD    | 107  | VAL  | 2.3  |
| 31  | BJ    | 64   | VAL  | 2.3  |
| 37  | DP    | 69   | VAL  | 2.3  |
| 41  | DT    | 79   | ASP  | 2.3  |
| 16  | CQ    | 62   | GLU  | 2.2  |
| 27  | BE    | 152  | GLU  | 2.2  |
| 1   | AA    | 410  | G    | 2.2  |
| 1   | AA    | 1020 | G    | 2.2  |
| 1   | CA    | 354  | G    | 2.2  |
| 1   | CA    | 812  | G    | 2.2  |
| 22  | DA    | 69   | G    | 2.2  |
| 23  | BB    | 1279 | G    | 2.2  |
| 23  | BB    | 2307 | G    | 2.2  |
| 23  | BB    | 2621 | G    | 2.2  |
| 23  | BB    | 2693 | G    | 2.2  |
| 23  | DB    | 75   | G    | 2.2  |
| 23  | DB    | 1388 | G    | 2.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 23  | DB    | 2630 | G    | 2.2  |
| 4   | AE    | 105  | ILE  | 2.2  |
| 32  | DK    | 47   | ILE  | 2.2  |
| 4   | CE    | 70   | MET  | 2.2  |
| 17  | AR    | 61   | ALA  | 2.2  |
| 34  | BM    | 29   | GLY  | 2.2  |
| 37  | DP    | 107  | ALA  | 2.2  |
| 52  | DI    | 82   | ALA  | 2.2  |
| 1   | AA    | 96   | U    | 2.2  |
| 1   | AA    | 228  | A    | 2.2  |
| 1   | AA    | 630  | A    | 2.2  |
| 1   | AA    | 1065 | U    | 2.2  |
| 1   | CA    | 672  | U    | 2.2  |
| 2   | CC    | 174  | LEU  | 2.2  |
| 9   | AJ    | 71   | LEU  | 2.2  |
| 20  | CB    | 134  | LEU  | 2.2  |
| 22  | DA    | 14   | U    | 2.2  |
| 22  | DA    | 99   | A    | 2.2  |
| 23  | BB    | 1101 | U    | 2.2  |
| 23  | BB    | 1434 | A    | 2.2  |
| 23  | BB    | 1786 | A    | 2.2  |
| 23  | BB    | 2340 | A    | 2.2  |
| 23  | BB    | 2687 | U    | 2.2  |
| 23  | DB    | 439  | A    | 2.2  |
| 23  | DB    | 1094 | U    | 2.2  |
| 23  | DB    | 1224 | U    | 2.2  |
| 23  | DB    | 2030 | A    | 2.2  |
| 23  | DB    | 2491 | U    | 2.2  |
| 46  | DZ    | 32   | LEU  | 2.2  |
| 8   | AI    | 83   | THR  | 2.2  |
| 9   | CJ    | 69   | THR  | 2.2  |
| 20  | CB    | 19   | THR  | 2.2  |
| 49  | D2    | 24   | THR  | 2.2  |
| 10  | AK    | 25   | SER  | 2.2  |
| 13  | CN    | 18   | LYS  | 2.2  |
| 13  | CN    | 54   | SER  | 2.2  |
| 13  | CN    | 97   | LYS  | 2.2  |
| 18  | CS    | 6    | LYS  | 2.2  |
| 19  | CT    | 7    | LYS  | 2.2  |
| 20  | CB    | 10   | LYS  | 2.2  |
| 25  | DC    | 110  | LYS  | 2.2  |
| 31  | DJ    | 39   | LYS  | 2.2  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 37  | DP    | 62   | LYS  | 2.2  |
| 47  | B0    | 48   | TYR  | 2.2  |
| 1   | AA    | 658  | C    | 2.2  |
| 1   | AA    | 1063 | C    | 2.2  |
| 1   | AA    | 1210 | C    | 2.2  |
| 1   | CA    | 962  | C    | 2.2  |
| 1   | CA    | 1320 | C    | 2.2  |
| 6   | CG    | 2    | ARG  | 2.2  |
| 12  | CM    | 97   | ARG  | 2.2  |
| 23  | BB    | 2870 | C    | 2.2  |
| 35  | DN    | 8    | ARG  | 2.2  |
| 36  | BO    | 30   | ARG  | 2.2  |
| 44  | BX    | 29   | ARG  | 2.2  |
| 6   | CG    | 27   | ASN  | 2.2  |
| 6   | CG    | 96   | ASN  | 2.2  |
| 10  | CK    | 14   | GLN  | 2.2  |
| 11  | AL    | 5    | GLN  | 2.2  |
| 16  | AQ    | 8    | GLN  | 2.2  |
| 16  | AQ    | 28   | VAL  | 2.2  |
| 26  | BD    | 107  | VAL  | 2.2  |
| 27  | DE    | 167  | VAL  | 2.2  |
| 31  | BJ    | 105  | VAL  | 2.2  |
| 33  | BL    | 4    | ASN  | 2.2  |
| 42  | DU    | 82   | VAL  | 2.2  |
| 46  | BZ    | 65   | ASN  | 2.2  |
| 48  | D1    | 11   | VAL  | 2.2  |
| 7   | CH    | 51   | GLU  | 2.2  |
| 24  | BV    | 69   | GLU  | 2.2  |
| 30  | BH    | 149  | GLU  | 2.2  |
| 34  | DM    | 75   | GLU  | 2.2  |
| 39  | DR    | 46   | GLU  | 2.2  |
| 48  | D1    | 31   | GLU  | 2.2  |
| 11  | AL    | 81   | ILE  | 2.2  |
| 35  | BN    | 113  | ILE  | 2.2  |
| 40  | DS    | 66   | ILE  | 2.2  |
| 2   | AC    | 123  | LEU  | 2.2  |
| 2   | CC    | 8    | GLY  | 2.2  |
| 9   | AJ    | 90   | LEU  | 2.2  |
| 9   | CJ    | 52   | LEU  | 2.2  |
| 11  | CL    | 67   | GLY  | 2.2  |
| 13  | AN    | 56   | PRO  | 2.2  |
| 21  | AU    | 10   | PRO  | 2.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 27  | DE    | 200  | LEU  | 2.2  |
| 30  | BH    | 106  | ALA  | 2.2  |
| 34  | BM    | 77   | PRO  | 2.2  |
| 32  | BK    | 25   | LEU  | 2.2  |
| 33  | DL    | 71   | ALA  | 2.2  |
| 35  | DN    | 77   | ALA  | 2.2  |
| 38  | BQ    | 6    | GLY  | 2.2  |
| 41  | BT    | 23   | ALA  | 2.2  |
| 1   | AA    | 134  | G    | 2.2  |
| 1   | CA    | 391  | G    | 2.2  |
| 8   | AI    | 114  | LYS  | 2.2  |
| 10  | AK    | 56   | LYS  | 2.2  |
| 13  | CN    | 96   | LYS  | 2.2  |
| 28  | BF    | 137  | PHE  | 2.2  |
| 27  | BE    | 43   | THR  | 2.2  |
| 28  | DF    | 34   | THR  | 2.2  |
| 31  | BJ    | 111  | LYS  | 2.2  |
| 32  | BK    | 40   | LYS  | 2.2  |
| 34  | DM    | 117  | PHE  | 2.2  |
| 14  | AO    | 49   | HIS  | 2.2  |
| 18  | AS    | 32   | THR  | 2.2  |
| 18  | AS    | 38   | THR  | 2.2  |
| 20  | AB    | 137  | THR  | 2.2  |
| 22  | DA    | 79   | G    | 2.2  |
| 23  | BB    | 2002 | G    | 2.2  |
| 23  | BB    | 2102 | G    | 2.2  |
| 23  | DB    | 1171 | G    | 2.2  |
| 23  | DB    | 2100 | G    | 2.2  |
| 23  | DB    | 2337 | G    | 2.2  |
| 23  | DB    | 2472 | G    | 2.2  |
| 23  | DB    | 2780 | G    | 2.2  |
| 26  | BD    | 51   | THR  | 2.2  |
| 39  | BR    | 66   | HIS  | 2.2  |
| 1   | AA    | 531  | U    | 2.2  |
| 1   | AA    | 1440 | U    | 2.2  |
| 1   | CA    | 485  | U    | 2.2  |
| 3   | AD    | 96   | ARG  | 2.2  |
| 6   | AG    | 43   | TYR  | 2.2  |
| 14  | AO    | 68   | TYR  | 2.2  |
| 23  | BB    | 1174 | U    | 2.2  |
| 23  | DB    | 2790 | U    | 2.2  |
| 25  | BC    | 61   | TYR  | 2.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 34  | BM    | 51   | ARG  | 2.2  |
| 35  | DN    | 96   | ARG  | 2.2  |
| 41  | DT    | 6    | ARG  | 2.2  |
| 1   | CA    | 974  | A    | 2.2  |
| 1   | CA    | 1044 | A    | 2.2  |
| 23  | BB    | 5    | A    | 2.2  |
| 23  | BB    | 933  | A    | 2.2  |
| 23  | DB    | 1089 | A    | 2.2  |
| 23  | DB    | 2211 | A    | 2.2  |
| 5   | CF    | 89   | VAL  | 2.2  |
| 24  | DV    | 47   | VAL  | 2.2  |
| 32  | BK    | 5    | GLN  | 2.2  |
| 49  | B2    | 29   | GLN  | 2.2  |
| 8   | CI    | 30   | ASN  | 2.2  |
| 20  | AB    | 145  | ASN  | 2.2  |
| 43  | DW    | 49   | ASN  | 2.2  |
| 46  | DZ    | 33   | ASN  | 2.2  |
| 4   | AE    | 115  | GLU  | 2.2  |
| 6   | CG    | 57   | GLU  | 2.2  |
| 10  | AK    | 115  | ILE  | 2.2  |
| 15  | AP    | 48   | GLU  | 2.2  |
| 20  | CB    | 163  | ILE  | 2.2  |
| 28  | BF    | 86   | CYS  | 2.2  |
| 42  | DU    | 38   | ILE  | 2.2  |
| 52  | BI    | 128  | ILE  | 2.2  |
| 1   | AA    | 1533 | C    | 2.2  |
| 1   | CA    | 1045 | C    | 2.2  |
| 16  | CQ    | 83   | LEU  | 2.2  |
| 19  | CT    | 58   | ASP  | 2.2  |
| 22  | BA    | 37   | C    | 2.2  |
| 23  | BB    | 1211 | C    | 2.2  |
| 23  | BB    | 2716 | C    | 2.2  |
| 23  | DB    | 1270 | C    | 2.2  |
| 23  | DB    | 1920 | C    | 2.2  |
| 12  | AM    | 80   | MET  | 2.2  |
| 14  | AO    | 65   | LEU  | 2.2  |
| 26  | BD    | 195  | GLY  | 2.2  |
| 27  | BE    | 39   | ALA  | 2.2  |
| 28  | BF    | 49   | LEU  | 2.2  |
| 32  | DK    | 12   | ASP  | 2.2  |
| 15  | AP    | 10   | GLY  | 2.2  |
| 24  | DV    | 27   | PRO  | 2.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 29  | BG    | 135 | ALA  | 2.2  |
| 37  | BP    | 21  | PRO  | 2.2  |
| 38  | DQ    | 66  | ALA  | 2.2  |
| 48  | B1    | 10  | LEU  | 2.2  |
| 49  | D2    | 1   | MET  | 2.2  |
| 52  | DI    | 62  | ALA  | 2.2  |
| 10  | AK    | 79  | LYS  | 2.2  |
| 11  | AL    | 17  | LYS  | 2.2  |
| 11  | AL    | 119 | LYS  | 2.2  |
| 15  | AP    | 12  | LYS  | 2.2  |
| 38  | DQ    | 53  | LYS  | 2.2  |
| 41  | BT    | 26  | LYS  | 2.2  |
| 45  | BY    | 18  | LYS  | 2.2  |
| 10  | CK    | 104 | PHE  | 2.2  |
| 28  | BF    | 174 | PHE  | 2.2  |
| 39  | BR    | 5   | PHE  | 2.2  |
| 8   | AI    | 94  | ARG  | 2.2  |
| 8   | AI    | 129 | ARG  | 2.2  |
| 8   | CI    | 32  | ARG  | 2.2  |
| 9   | CJ    | 48  | ARG  | 2.2  |
| 10  | AK    | 55  | ARG  | 2.2  |
| 11  | CL    | 8   | ARG  | 2.2  |
| 49  | D2    | 39  | ARG  | 2.2  |
| 9   | CJ    | 70  | HIS  | 2.2  |
| 35  | BN    | 37  | THR  | 2.2  |
| 2   | AC    | 172 | VAL  | 2.2  |
| 3   | CD    | 24  | VAL  | 2.2  |
| 14  | AO    | 59  | VAL  | 2.2  |
| 15  | AP    | 20  | VAL  | 2.2  |
| 19  | AT    | 5   | SER  | 2.2  |
| 38  | DQ    | 74  | SER  | 2.2  |
| 42  | BU    | 67  | SER  | 2.2  |
| 1   | AA    | 562 | U    | 2.2  |
| 1   | AA    | 723 | U    | 2.2  |
| 1   | CA    | 438 | U    | 2.2  |
| 48  | B1    | 44  | GLN  | 2.2  |
| 52  | BI    | 11  | GLN  | 2.2  |
| 16  | AQ    | 20  | ILE  | 2.2  |
| 20  | CB    | 185 | ILE  | 2.2  |
| 28  | DF    | 110 | ILE  | 2.2  |
| 34  | BM    | 73  | ILE  | 2.2  |
| 37  | BP    | 83  | ILE  | 2.2  |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 50         | D3           | 58         | ILE         | 2.2         |
| 1          | AA           | 502        | A           | 2.2         |
| 1          | AA           | 946        | A           | 2.2         |
| 1          | AA           | 1000       | A           | 2.2         |
| 1          | AA           | 1150       | A           | 2.2         |
| 1          | AA           | 1280       | A           | 2.2         |
| 1          | AA           | 1297       | G           | 2.2         |
| 1          | AA           | 1519       | A           | 2.2         |
| 1          | CA           | 725        | G           | 2.2         |
| 1          | CA           | 1215       | G           | 2.2         |
| 23         | BB           | 1051       | G           | 2.2         |
| 23         | BB           | 1327       | A           | 2.2         |
| 23         | BB           | 1610       | A           | 2.2         |
| 23         | BB           | 2060       | A           | 2.2         |
| 23         | BB           | 2287       | A           | 2.2         |
| 23         | BB           | 2523       | G           | 2.2         |
| 23         | BB           | 2668       | G           | 2.2         |
| 23         | DB           | 227        | A           | 2.2         |
| 23         | DB           | 232        | G           | 2.2         |
| 23         | DB           | 474        | G           | 2.2         |
| 23         | DB           | 973        | A           | 2.2         |
| 23         | DB           | 1490       | A           | 2.2         |
| 23         | DB           | 1888       | G           | 2.2         |
| 3          | AD           | 10         | LEU         | 2.2         |
| 7          | AH           | 39         | LEU         | 2.2         |
| 8          | AI           | 62         | LEU         | 2.2         |
| 12         | AM           | 74         | MET         | 2.2         |
| 12         | CM           | 80         | MET         | 2.2         |
| 18         | AS           | 43         | MET         | 2.2         |
| 23         | DB           | 2883       | A           | 2.2         |
| 29         | BG           | 36         | LEU         | 2.2         |
| 38         | BQ           | 108        | LEU         | 2.2         |
| 46         | DZ           | 34         | LEU         | 2.2         |
| 6          | CG           | 13         | PRO         | 2.2         |
| 9          | AJ           | 79         | PRO         | 2.2         |
| 19         | AT           | 40         | ALA         | 2.2         |
| 27         | BE           | 68         | ALA         | 2.2         |
| 27         | DE           | 20         | GLY         | 2.2         |
| 29         | DG           | 7          | PRO         | 2.2         |
| 29         | DG           | 45         | ALA         | 2.2         |
| 31         | BJ           | 107        | GLY         | 2.2         |
| 36         | DO           | 6          | ALA         | 2.2         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 52  | DI    | 116  | MET  | 2.2  |
| 20  | AB    | 24   | PRO  | 2.2  |
| 24  | DV    | 37   | PRO  | 2.2  |
| 25  | DC    | 135  | PRO  | 2.2  |
| 38  | BQ    | 81   | GLY  | 2.2  |
| 42  | DU    | 49   | PRO  | 2.2  |
| 46  | BZ    | 55   | GLY  | 2.2  |
| 2   | AC    | 82   | ASP  | 2.2  |
| 2   | AC    | 180  | ASP  | 2.2  |
| 3   | CD    | 30   | LYS  | 2.2  |
| 8   | CI    | 61   | ASP  | 2.2  |
| 16  | CQ    | 15   | LYS  | 2.2  |
| 24  | DV    | 25   | LYS  | 2.2  |
| 27  | BE    | 47   | LYS  | 2.2  |
| 27  | BE    | 168  | ASP  | 2.2  |
| 41  | BT    | 68   | LYS  | 2.2  |
| 46  | DZ    | 23   | LYS  | 2.2  |
| 4   | AE    | 47   | PHE  | 2.2  |
| 9   | AJ    | 31   | ARG  | 2.2  |
| 9   | AJ    | 62   | ARG  | 2.2  |
| 28  | BF    | 19   | PHE  | 2.2  |
| 28  | DF    | 109  | ARG  | 2.2  |
| 32  | BK    | 30   | ARG  | 2.2  |
| 35  | DN    | 67   | PHE  | 2.2  |
| 1   | AA    | 984  | C    | 2.2  |
| 1   | AA    | 1217 | C    | 2.2  |
| 1   | AA    | 1226 | C    | 2.2  |
| 1   | AA    | 1296 | C    | 2.2  |
| 23  | BB    | 560  | C    | 2.2  |
| 23  | BB    | 2422 | C    | 2.2  |
| 23  | DB    | 128  | C    | 2.2  |
| 23  | DB    | 385  | C    | 2.2  |
| 23  | DB    | 2150 | C    | 2.2  |
| 18  | CS    | 13   | HIS  | 2.2  |
| 25  | DC    | 245  | THR  | 2.2  |
| 27  | BE    | 84   | THR  | 2.2  |
| 28  | DF    | 154  | THR  | 2.2  |
| 37  | DP    | 103  | THR  | 2.2  |
| 52  | BI    | 111  | THR  | 2.2  |
| 3   | AD    | 75   | TYR  | 2.2  |
| 7   | CH    | 33   | VAL  | 2.2  |
| 8   | AI    | 115  | VAL  | 2.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 18  | AS    | 59   | VAL  | 2.2  |
| 18  | CS    | 66   | VAL  | 2.2  |
| 25  | BC    | 171  | VAL  | 2.2  |
| 28  | BF    | 12   | VAL  | 2.2  |
| 36  | DO    | 47   | VAL  | 2.2  |
| 30  | BH    | 80   | ILE  | 2.2  |
| 31  | BJ    | 135  | GLN  | 2.2  |
| 34  | DM    | 96   | ILE  | 2.2  |
| 50  | B3    | 31   | ILE  | 2.2  |
| 13  | AN    | 47   | LEU  | 2.2  |
| 49  | B2    | 42   | LEU  | 2.2  |
| 2   | CC    | 133  | MET  | 2.2  |
| 7   | AH    | 114  | ALA  | 2.2  |
| 7   | AH    | 115  | ALA  | 2.2  |
| 27  | DE    | 45   | ALA  | 2.2  |
| 26  | DD    | 44   | GLY  | 2.2  |
| 29  | BG    | 171  | LYS  | 2.2  |
| 31  | BJ    | 131  | ASN  | 2.2  |
| 42  | DU    | 52   | ASN  | 2.2  |
| 44  | BX    | 59   | GLU  | 2.2  |
| 44  | DX    | 5    | GLU  | 2.2  |
| 1   | AA    | 409  | U    | 2.2  |
| 1   | AA    | 1528 | U    | 2.2  |
| 12  | CM    | 110  | GLY  | 2.2  |
| 13  | AN    | 18   | LYS  | 2.2  |
| 15  | CP    | 76   | LYS  | 2.2  |
| 19  | CT    | 84   | LYS  | 2.2  |
| 44  | DX    | 15   | ASN  | 2.2  |
| 23  | BB    | 1060 | U    | 2.2  |
| 23  | DB    | 807  | U    | 2.2  |
| 23  | DB    | 1082 | U    | 2.2  |
| 39  | BR    | 8    | GLY  | 2.2  |
| 52  | DI    | 55   | PRO  | 2.2  |
| 4   | CE    | 53   | ARG  | 2.2  |
| 10  | AK    | 127  | ARG  | 2.2  |
| 28  | BF    | 91   | ARG  | 2.2  |
| 29  | BG    | 34   | ARG  | 2.2  |
| 32  | BK    | 31   | ARG  | 2.2  |
| 11  | AL    | 102  | ASP  | 2.2  |
| 20  | AB    | 161  | PHE  | 2.2  |
| 27  | DE    | 85   | PHE  | 2.2  |
| 32  | DK    | 56   | ASP  | 2.2  |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 34         | DM           | 25         | ASP         | 2.2         |
| 1          | AA           | 250        | A           | 2.2         |
| 1          | AA           | 949        | A           | 2.2         |
| 1          | AA           | 1101       | A           | 2.2         |
| 1          | CA           | 1287       | A           | 2.2         |
| 23         | BB           | 528        | A           | 2.2         |
| 23         | BB           | 2212       | A           | 2.2         |
| 23         | BB           | 2657       | A           | 2.2         |
| 23         | BB           | 2761       | A           | 2.2         |
| 23         | DB           | 348        | A           | 2.2         |
| 23         | DB           | 1073       | A           | 2.2         |
| 23         | DB           | 1434       | A           | 2.2         |
| 23         | DB           | 2090       | A           | 2.2         |
| 23         | DB           | 2199       | A           | 2.2         |
| 1          | AA           | 6          | G           | 2.2         |
| 1          | AA           | 147        | G           | 2.2         |
| 1          | AA           | 567        | G           | 2.2         |
| 1          | AA           | 730        | G           | 2.2         |
| 1          | CA           | 164        | G           | 2.2         |
| 23         | BB           | 1897       | G           | 2.2         |
| 23         | BB           | 2012       | G           | 2.2         |
| 23         | BB           | 2152       | G           | 2.2         |
| 23         | BB           | 2719       | G           | 2.2         |
| 23         | DB           | 215        | G           | 2.2         |
| 23         | DB           | 1087       | G           | 2.2         |
| 27         | DE           | 29         | HIS         | 2.2         |
| 3          | AD           | 200        | VAL         | 2.1         |
| 8          | AI           | 65         | THR         | 2.1         |
| 10         | CK           | 45         | THR         | 2.1         |
| 14         | CO           | 21         | THR         | 2.1         |
| 28         | BF           | 73         | VAL         | 2.1         |
| 30         | DH           | 130        | VAL         | 2.1         |
| 31         | DJ           | 45         | THR         | 2.1         |
| 38         | DQ           | 30         | VAL         | 2.1         |
| 41         | BT           | 34         | VAL         | 2.1         |
| 24         | DV           | 57         | TYR         | 2.1         |
| 1          | AA           | 40         | C           | 2.1         |
| 1          | AA           | 489        | C           | 2.1         |
| 1          | AA           | 511        | C           | 2.1         |
| 1          | CA           | 469        | C           | 2.1         |
| 1          | CA           | 1129       | C           | 2.1         |
| 2          | CC           | 206        | ILE         | 2.1         |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 22  | DA    | 26   | C    | 2.1  |
| 22  | DA    | 60   | C    | 2.1  |
| 23  | BB    | 994  | C    | 2.1  |
| 23  | BB    | 1606 | C    | 2.1  |
| 23  | DB    | 1493 | C    | 2.1  |
| 30  | BH    | 4    | ILE  | 2.1  |
| 31  | BJ    | 54   | ILE  | 2.1  |
| 48  | D1    | 53   | ILE  | 2.1  |
| 4   | AE    | 81   | GLN  | 2.1  |
| 10  | CK    | 81   | LEU  | 2.1  |
| 12  | AM    | 99   | GLN  | 2.1  |
| 15  | CP    | 63   | GLN  | 2.1  |
| 27  | DE    | 94   | GLN  | 2.1  |
| 28  | BF    | 80   | GLN  | 2.1  |
| 33  | DL    | 19   | LEU  | 2.1  |
| 44  | BX    | 6    | LEU  | 2.1  |
| 4   | AE    | 22   | LYS  | 2.1  |
| 2   | AC    | 29   | ALA  | 2.1  |
| 7   | CH    | 22   | ALA  | 2.1  |
| 11  | CL    | 123  | ALA  | 2.1  |
| 13  | AN    | 21   | ALA  | 2.1  |
| 25  | BC    | 177  | SER  | 2.1  |
| 27  | BE    | 106  | LYS  | 2.1  |
| 28  | DF    | 37   | MET  | 2.1  |
| 29  | DG    | 5    | LYS  | 2.1  |
| 34  | BM    | 133  | LYS  | 2.1  |
| 35  | DN    | 35   | LYS  | 2.1  |
| 50  | D3    | 51   | LYS  | 2.1  |
| 2   | CC    | 1    | GLY  | 2.1  |
| 6   | AG    | 101  | ARG  | 2.1  |
| 4   | AE    | 131  | ASN  | 2.1  |
| 8   | CI    | 22   | PRO  | 2.1  |
| 11  | CL    | 82   | ARG  | 2.1  |
| 25  | DC    | 78   | GLU  | 2.1  |
| 26  | DD    | 71   | ALA  | 2.1  |
| 31  | BJ    | 104  | ALA  | 2.1  |
| 33  | BL    | 72   | ALA  | 2.1  |
| 33  | DL    | 15   | ALA  | 2.1  |
| 15  | AP    | 41   | PRO  | 2.1  |
| 25  | DC    | 98   | GLY  | 2.1  |
| 25  | DC    | 132  | ARG  | 2.1  |
| 38  | DQ    | 27   | ARG  | 2.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 39  | BR    | 62   | GLU  | 2.1  |
| 39  | DR    | 21   | ARG  | 2.1  |
| 39  | DR    | 34   | GLU  | 2.1  |
| 26  | BD    | 120  | GLY  | 2.1  |
| 26  | DD    | 63   | PRO  | 2.1  |
| 27  | DE    | 76   | PRO  | 2.1  |
| 29  | BG    | 11   | PRO  | 2.1  |
| 30  | BH    | 85   | GLY  | 2.1  |
| 31  | BJ    | 8    | PRO  | 2.1  |
| 31  | DJ    | 131  | ASN  | 2.1  |
| 44  | DX    | 20   | ASN  | 2.1  |
| 4   | CE    | 30   | PHE  | 2.1  |
| 19  | CT    | 30   | PHE  | 2.1  |
| 20  | CB    | 90   | PHE  | 2.1  |
| 1   | CA    | 390  | U    | 2.1  |
| 1   | CA    | 1211 | U    | 2.1  |
| 1   | CA    | 1364 | U    | 2.1  |
| 11  | CL    | 88   | ASP  | 2.1  |
| 14  | AO    | 17   | ASP  | 2.1  |
| 22  | BA    | 80   | U    | 2.1  |
| 23  | BB    | 339  | U    | 2.1  |
| 23  | BB    | 1466 | U    | 2.1  |
| 23  | DB    | 50   | U    | 2.1  |
| 23  | DB    | 2387 | U    | 2.1  |
| 2   | CC    | 14   | VAL  | 2.1  |
| 37  | BP    | 45   | VAL  | 2.1  |
| 47  | D0    | 41   | HIS  | 2.1  |
| 20  | CB    | 124  | THR  | 2.1  |
| 20  | CB    | 129  | THR  | 2.1  |
| 1   | AA    | 452  | A    | 2.1  |
| 1   | AA    | 1067 | A    | 2.1  |
| 2   | AC    | 119  | ILE  | 2.1  |
| 3   | AD    | 203  | TYR  | 2.1  |
| 5   | CF    | 59   | TYR  | 2.1  |
| 9   | CJ    | 18   | ILE  | 2.1  |
| 23  | BB    | 1070 | A    | 2.1  |
| 23  | BB    | 2560 | A    | 2.1  |
| 23  | DB    | 1981 | A    | 2.1  |
| 40  | DS    | 96   | ILE  | 2.1  |
| 42  | DU    | 102  | ILE  | 2.1  |
| 6   | CG    | 119  | LEU  | 2.1  |
| 7   | CH    | 32   | LYS  | 2.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 9   | AJ    | 82   | LYS  | 2.1  |
| 27  | BE    | 147  | LEU  | 2.1  |
| 30  | DH    | 22   | LYS  | 2.1  |
| 41  | BT    | 11   | LEU  | 2.1  |
| 52  | DI    | 137  | LEU  | 2.1  |
| 1   | AA    | 46   | G    | 2.1  |
| 1   | AA    | 165  | G    | 2.1  |
| 1   | AA    | 818  | G    | 2.1  |
| 1   | AA    | 947  | G    | 2.1  |
| 1   | CA    | 108  | G    | 2.1  |
| 1   | CA    | 849  | G    | 2.1  |
| 1   | CA    | 1276 | G    | 2.1  |
| 3   | AD    | 153  | ARG  | 2.1  |
| 9   | CJ    | 35   | GLN  | 2.1  |
| 11  | AL    | 85   | ARG  | 2.1  |
| 18  | CS    | 80   | ARG  | 2.1  |
| 23  | BB    | 258  | G    | 2.1  |
| 23  | BB    | 808  | G    | 2.1  |
| 23  | BB    | 1651 | G    | 2.1  |
| 23  | BB    | 2535 | G    | 2.1  |
| 23  | BB    | 2640 | G    | 2.1  |
| 23  | BB    | 2641 | G    | 2.1  |
| 23  | BB    | 2659 | G    | 2.1  |
| 23  | DB    | 549  | G    | 2.1  |
| 23  | DB    | 1192 | G    | 2.1  |
| 23  | DB    | 1324 | G    | 2.1  |
| 23  | DB    | 1581 | G    | 2.1  |
| 23  | DB    | 1921 | G    | 2.1  |
| 23  | DB    | 2869 | G    | 2.1  |
| 27  | DE    | 46   | GLN  | 2.1  |
| 28  | DF    | 132  | ARG  | 2.1  |
| 33  | DL    | 104  | GLN  | 2.1  |
| 39  | BR    | 40   | MET  | 2.1  |
| 20  | CB    | 184  | ALA  | 2.1  |
| 21  | CU    | 47   | ALA  | 2.1  |
| 30  | BH    | 105  | ALA  | 2.1  |
| 31  | BJ    | 6    | ALA  | 2.1  |
| 32  | DK    | 83   | ALA  | 2.1  |
| 47  | B0    | 51   | ARG  | 2.1  |
| 47  | B0    | 55   | ALA  | 2.1  |
| 50  | B3    | 10   | ALA  | 2.1  |
| 10  | AK    | 54   | SER  | 2.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 19  | CT    | 5    | SER  | 2.1  |
| 28  | BF    | 117  | SER  | 2.1  |
| 30  | BH    | 76   | GLU  | 2.1  |
| 33  | DL    | 114  | GLY  | 2.1  |
| 36  | BO    | 20   | GLU  | 2.1  |
| 43  | DW    | 53   | GLY  | 2.1  |
| 1   | AA    | 99   | C    | 2.1  |
| 23  | BB    | 1833 | C    | 2.1  |
| 23  | BB    | 2681 | C    | 2.1  |
| 10  | CK    | 51   | PHE  | 2.1  |
| 26  | DD    | 15   | PHE  | 2.1  |
| 2   | AC    | 75   | VAL  | 2.1  |
| 7   | CH    | 103  | VAL  | 2.1  |
| 12  | AM    | 53   | ASP  | 2.1  |
| 20  | CB    | 196  | ASP  | 2.1  |
| 28  | DF    | 27   | VAL  | 2.1  |
| 29  | BG    | 75   | VAL  | 2.1  |
| 32  | BK    | 24   | VAL  | 2.1  |
| 3   | CD    | 40   | HIS  | 2.1  |
| 3   | CD    | 119  | HIS  | 2.1  |
| 25  | BC    | 229  | HIS  | 2.1  |
| 1   | AA    | 88   | U    | 2.1  |
| 1   | AA    | 1512 | U    | 2.1  |
| 1   | CA    | 1030 | U    | 2.1  |
| 3   | AD    | 9    | LYS  | 2.1  |
| 5   | AF    | 56   | LYS  | 2.1  |
| 7   | CH    | 74   | ILE  | 2.1  |
| 12  | CM    | 101  | THR  | 2.1  |
| 18  | CS    | 70   | LEU  | 2.1  |
| 20  | AB    | 116  | LEU  | 2.1  |
| 23  | BB    | 206  | U    | 2.1  |
| 23  | BB    | 1033 | U    | 2.1  |
| 24  | BV    | 38   | LEU  | 2.1  |
| 25  | BC    | 149  | LYS  | 2.1  |
| 25  | BC    | 201  | LEU  | 2.1  |
| 25  | DC    | 173  | LEU  | 2.1  |
| 26  | BD    | 160  | LYS  | 2.1  |
| 27  | BE    | 13   | THR  | 2.1  |
| 27  | DE    | 164  | LEU  | 2.1  |
| 28  | DF    | 178  | LYS  | 2.1  |
| 29  | BG    | 120  | ILE  | 2.1  |
| 33  | BL    | 79   | LEU  | 2.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 35  | DN    | 70   | THR  | 2.1  |
| 40  | BS    | 72   | THR  | 2.1  |
| 43  | DW    | 81   | ILE  | 2.1  |
| 47  | D0    | 11   | LYS  | 2.1  |
| 50  | B3    | 33   | THR  | 2.1  |
| 52  | DI    | 128  | ILE  | 2.1  |
| 3   | AD    | 2    | ARG  | 2.1  |
| 10  | CK    | 52   | ARG  | 2.1  |
| 35  | BN    | 110  | MET  | 2.1  |
| 36  | BO    | 25   | ARG  | 2.1  |
| 36  | DO    | 94   | ARG  | 2.1  |
| 46  | DZ    | 56   | ARG  | 2.1  |
| 6   | AG    | 144  | ALA  | 2.1  |
| 27  | DE    | 41   | GLN  | 2.1  |
| 27  | DE    | 136  | GLN  | 2.1  |
| 34  | BM    | 122  | ALA  | 2.1  |
| 52  | BI    | 26   | ALA  | 2.1  |
| 1   | AA    | 223  | A    | 2.1  |
| 1   | AA    | 364  | A    | 2.1  |
| 1   | CA    | 143  | A    | 2.1  |
| 1   | CA    | 411  | A    | 2.1  |
| 2   | AC    | 170  | GLY  | 2.1  |
| 3   | CD    | 159  | GLU  | 2.1  |
| 7   | CH    | 43   | GLY  | 2.1  |
| 13  | CN    | 77   | GLY  | 2.1  |
| 13  | CN    | 94   | GLY  | 2.1  |
| 23  | BB    | 981  | A    | 2.1  |
| 23  | BB    | 2883 | A    | 2.1  |
| 23  | DB    | 1048 | A    | 2.1  |
| 23  | DB    | 1640 | A    | 2.1  |
| 23  | DB    | 2031 | A    | 2.1  |
| 25  | BC    | 106  | PRO  | 2.1  |
| 25  | BC    | 108  | GLY  | 2.1  |
| 25  | DC    | 40   | GLY  | 2.1  |
| 25  | DC    | 226  | PRO  | 2.1  |
| 28  | DF    | 85   | GLY  | 2.1  |
| 29  | DG    | 141  | GLY  | 2.1  |
| 43  | BW    | 41   | GLY  | 2.1  |
| 44  | DX    | 12   | GLU  | 2.1  |
| 18  | CS    | 9    | PHE  | 2.1  |
| 29  | BG    | 109  | SER  | 2.1  |
| 39  | BR    | 15   | SER  | 2.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 52  | DI    | 20   | SER  | 2.1  |
| 34  | DM    | 88   | ASN  | 2.1  |
| 35  | DN    | 13   | ASN  | 2.1  |
| 1   | AA    | 142  | G    | 2.1  |
| 1   | AA    | 350  | G    | 2.1  |
| 1   | AA    | 455  | G    | 2.1  |
| 1   | AA    | 570  | G    | 2.1  |
| 1   | AA    | 1305 | G    | 2.1  |
| 1   | CA    | 1190 | G    | 2.1  |
| 1   | CA    | 1300 | G    | 2.1  |
| 14  | CO    | 11   | VAL  | 2.1  |
| 23  | BB    | 745  | G    | 2.1  |
| 23  | BB    | 805  | G    | 2.1  |
| 23  | BB    | 1737 | G    | 2.1  |
| 23  | BB    | 2341 | G    | 2.1  |
| 23  | DB    | 1455 | G    | 2.1  |
| 28  | BF    | 88   | VAL  | 2.1  |
| 29  | DG    | 14   | VAL  | 2.1  |
| 39  | DR    | 20   | VAL  | 2.1  |
| 1   | AA    | 334  | C    | 2.1  |
| 1   | AA    | 1137 | C    | 2.1  |
| 1   | CA    | 1158 | C    | 2.1  |
| 23  | BB    | 267  | C    | 2.1  |
| 3   | AD    | 184  | LYS  | 2.1  |
| 3   | CD    | 9    | LYS  | 2.1  |
| 3   | CD    | 21   | LYS  | 2.1  |
| 8   | CI    | 67   | LYS  | 2.1  |
| 5   | AF    | 22   | ILE  | 2.1  |
| 7   | AH    | 100  | ILE  | 2.1  |
| 9   | CJ    | 91   | ASP  | 2.1  |
| 39  | BR    | 76   | LYS  | 2.1  |
| 21  | AU    | 22   | CYS  | 2.1  |
| 25  | DC    | 32   | LEU  | 2.1  |
| 42  | DU    | 4    | ILE  | 2.1  |
| 44  | BX    | 37   | LEU  | 2.1  |
| 46  | DZ    | 12   | ILE  | 2.1  |
| 13  | CN    | 12   | ARG  | 2.1  |
| 25  | DC    | 237  | ARG  | 2.1  |
| 26  | DD    | 35   | THR  | 2.1  |
| 29  | DG    | 48   | THR  | 2.1  |
| 34  | DM    | 51   | ARG  | 2.1  |
| 2   | CC    | 128  | MET  | 2.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | AD    | 26   | ALA  | 2.1  |
| 3   | AD    | 156  | ALA  | 2.1  |
| 16  | CQ    | 81   | ALA  | 2.1  |
| 27  | BE    | 11   | ALA  | 2.1  |
| 30  | DH    | 36   | ALA  | 2.1  |
| 34  | DM    | 94   | ALA  | 2.1  |
| 1   | CA    | 950  | U    | 2.1  |
| 2   | AC    | 138  | GLN  | 2.1  |
| 23  | BB    | 562  | U    | 2.1  |
| 23  | BB    | 1267 | U    | 2.1  |
| 23  | BB    | 2514 | U    | 2.1  |
| 23  | DB    | 369  | U    | 2.1  |
| 25  | BC    | 116  | GLN  | 2.1  |
| 30  | BH    | 18   | GLN  | 2.1  |
| 49  | D2    | 29   | GLN  | 2.1  |
| 52  | BI    | 30   | GLN  | 2.1  |
| 3   | AD    | 105  | GLY  | 2.1  |
| 4   | AE    | 41   | GLY  | 2.1  |
| 33  | DL    | 24   | GLY  | 2.1  |
| 34  | DM    | 39   | GLY  | 2.1  |
| 2   | AC    | 109  | GLU  | 2.1  |
| 4   | CE    | 9    | GLU  | 2.1  |
| 6   | AG    | 150  | PHE  | 2.1  |
| 7   | CH    | 44   | PHE  | 2.1  |
| 11  | CL    | 44   | PRO  | 2.1  |
| 14  | AO    | 44   | GLU  | 2.1  |
| 15  | CP    | 15   | PRO  | 2.1  |
| 20  | AB    | 125  | PHE  | 2.1  |
| 20  | AB    | 144  | GLU  | 2.1  |
| 31  | BJ    | 113  | PRO  | 2.1  |
| 32  | DK    | 45   | GLU  | 2.1  |
| 39  | BR    | 53   | PHE  | 2.1  |
| 26  | DD    | 21   | SER  | 2.1  |
| 29  | BG    | 105  | SER  | 2.1  |
| 38  | BQ    | 86   | SER  | 2.1  |
| 2   | AC    | 137  | VAL  | 2.1  |
| 6   | AG    | 140  | VAL  | 2.1  |
| 7   | AH    | 109  | VAL  | 2.1  |
| 27  | DE    | 32   | VAL  | 2.1  |
| 41  | BT    | 96   | VAL  | 2.1  |
| 1   | AA    | 44   | A    | 2.1  |
| 1   | AA    | 482  | A    | 2.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | AA    | 1092 | A    | 2.1  |
| 1   | AA    | 1110 | A    | 2.1  |
| 1   | AA    | 1261 | A    | 2.1  |
| 1   | CA    | 171  | A    | 2.1  |
| 9   | CJ    | 11   | LYS  | 2.1  |
| 10  | CK    | 124  | LYS  | 2.1  |
| 23  | BB    | 218  | A    | 2.1  |
| 23  | BB    | 422  | A    | 2.1  |
| 23  | DB    | 152  | A    | 2.1  |
| 23  | DB    | 514  | A    | 2.1  |
| 23  | DB    | 643  | A    | 2.1  |
| 23  | DB    | 2589 | A    | 2.1  |
| 31  | DJ    | 106  | LYS  | 2.1  |
| 36  | BO    | 4    | LYS  | 2.1  |
| 44  | BX    | 15   | ASN  | 2.1  |
| 50  | B3    | 27   | ASN  | 2.1  |
| 52  | DI    | 91   | LYS  | 2.1  |
| 2   | CC    | 11   | LEU  | 2.1  |
| 3   | CD    | 158  | LEU  | 2.1  |
| 4   | CE    | 104  | ILE  | 2.1  |
| 25  | BC    | 13   | ARG  | 2.1  |
| 26  | BD    | 59   | ARG  | 2.1  |
| 27  | BE    | 170  | ARG  | 2.1  |
| 34  | DM    | 41   | LEU  | 2.1  |
| 34  | DM    | 66   | ARG  | 2.1  |
| 35  | DN    | 22   | ARG  | 2.1  |
| 41  | DT    | 11   | LEU  | 2.1  |
| 47  | B0    | 42   | ILE  | 2.1  |
| 5   | AF    | 90   | MET  | 2.1  |
| 8   | AI    | 55   | ASP  | 2.1  |
| 26  | DD    | 103  | ASP  | 2.1  |
| 28  | DF    | 9    | ASP  | 2.1  |
| 30  | BH    | 17   | ASP  | 2.1  |
| 11  | AL    | 103  | CYS  | 2.1  |
| 14  | CO    | 68   | TYR  | 2.1  |
| 25  | BC    | 170  | TYR  | 2.1  |
| 26  | DD    | 45   | TYR  | 2.1  |
| 28  | DF    | 6    | TYR  | 2.1  |
| 1   | AA    | 631  | C    | 2.1  |
| 1   | AA    | 651  | C    | 2.1  |
| 1   | AA    | 726  | C    | 2.1  |
| 1   | AA    | 1277 | C    | 2.1  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | CA    | 83   | C    | 2.1  |
| 1   | CA    | 1054 | C    | 2.1  |
| 1   | AA    | 587  | G    | 2.1  |
| 1   | CA    | 1361 | G    | 2.1  |
| 5   | AF    | 66   | ALA  | 2.1  |
| 18  | AS    | 21   | ALA  | 2.1  |
| 19  | AT    | 10   | ALA  | 2.1  |
| 19  | CT    | 37   | ALA  | 2.1  |
| 19  | CT    | 86   | ALA  | 2.1  |
| 23  | BB    | 140  | C    | 2.1  |
| 23  | BB    | 143  | C    | 2.1  |
| 23  | BB    | 490  | C    | 2.1  |
| 23  | BB    | 1493 | C    | 2.1  |
| 23  | BB    | 1625 | C    | 2.1  |
| 23  | BB    | 2717 | C    | 2.1  |
| 23  | BB    | 2794 | C    | 2.1  |
| 23  | DB    | 1607 | C    | 2.1  |
| 23  | DB    | 2551 | C    | 2.1  |
| 23  | BB    | 1071 | G    | 2.1  |
| 23  | BB    | 1136 | G    | 2.1  |
| 23  | BB    | 1187 | G    | 2.1  |
| 23  | BB    | 1339 | G    | 2.1  |
| 23  | BB    | 1343 | G    | 2.1  |
| 23  | BB    | 2107 | G    | 2.1  |
| 23  | BB    | 2136 | G    | 2.1  |
| 23  | BB    | 2867 | G    | 2.1  |
| 23  | DB    | 648  | G    | 2.1  |
| 23  | DB    | 997  | G    | 2.1  |
| 23  | DB    | 1187 | G    | 2.1  |
| 23  | DB    | 1212 | G    | 2.1  |
| 23  | DB    | 1216 | G    | 2.1  |
| 23  | DB    | 1424 | G    | 2.1  |
| 23  | DB    | 1723 | G    | 2.1  |
| 33  | DL    | 133  | ALA  | 2.1  |
| 35  | DN    | 104  | ALA  | 2.1  |
| 52  | DI    | 40   | ALA  | 2.1  |
| 8   | CI    | 125  | GLN  | 2.1  |
| 11  | AL    | 83   | GLY  | 2.1  |
| 38  | DQ    | 36   | GLN  | 2.1  |
| 41  | BT    | 90   | GLY  | 2.1  |
| 47  | B0    | 13   | GLY  | 2.1  |
| 8   | CI    | 91   | GLU  | 2.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 9   | CJ    | 55   | PRO  | 2.1  |
| 33  | DL    | 10   | GLU  | 2.1  |
| 1   | AA    | 14   | U    | 2.0  |
| 1   | AA    | 842  | U    | 2.0  |
| 7   | AH    | 32   | LYS  | 2.0  |
| 18  | AS    | 17   | LYS  | 2.0  |
| 23  | BB    | 2151 | U    | 2.0  |
| 23  | BB    | 2181 | U    | 2.0  |
| 23  | BB    | 2493 | U    | 2.0  |
| 23  | BB    | 2871 | U    | 2.0  |
| 23  | DB    | 811  | U    | 2.0  |
| 23  | DB    | 2479 | U    | 2.0  |
| 30  | DH    | 8    | LYS  | 2.0  |
| 35  | DN    | 42   | LYS  | 2.0  |
| 38  | BQ    | 30   | VAL  | 2.0  |
| 39  | BR    | 38   | VAL  | 2.0  |
| 39  | BR    | 54   | VAL  | 2.0  |
| 13  | AN    | 31   | SER  | 2.0  |
| 28  | DF    | 60   | SER  | 2.0  |
| 30  | BH    | 113  | SER  | 2.0  |
| 37  | BP    | 84   | SER  | 2.0  |
| 6   | AG    | 69   | ARG  | 2.0  |
| 7   | CH    | 124  | ILE  | 2.0  |
| 13  | CN    | 50   | LEU  | 2.0  |
| 18  | AS    | 52   | ASN  | 2.0  |
| 21  | AU    | 20   | ARG  | 2.0  |
| 26  | BD    | 40   | LEU  | 2.0  |
| 30  | DH    | 27   | ARG  | 2.0  |
| 30  | DH    | 97   | ARG  | 2.0  |
| 33  | DL    | 79   | LEU  | 2.0  |
| 35  | BN    | 73   | ASN  | 2.0  |
| 37  | DP    | 88   | ARG  | 2.0  |
| 42  | BU    | 21   | ARG  | 2.0  |
| 43  | BW    | 54   | ARG  | 2.0  |
| 49  | B2    | 26   | ASN  | 2.0  |
| 8   | AI    | 37   | TYR  | 2.0  |
| 8   | CI    | 107  | ALA  | 2.0  |
| 10  | CK    | 46   | ALA  | 2.0  |
| 12  | AM    | 107  | THR  | 2.0  |
| 14  | AO    | 8    | ALA  | 2.0  |
| 14  | CO    | 32   | THR  | 2.0  |
| 17  | CR    | 22   | TYR  | 2.0  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 22  | BA    | 78   | A    | 2.0  |
| 23  | BB    | 1359 | A    | 2.0  |
| 23  | BB    | 1616 | A    | 2.0  |
| 23  | BB    | 2516 | A    | 2.0  |
| 23  | BB    | 2887 | A    | 2.0  |
| 26  | BD    | 102  | ALA  | 2.0  |
| 26  | BD    | 151  | THR  | 2.0  |
| 28  | DF    | 118  | ALA  | 2.0  |
| 30  | DH    | 7    | ASP  | 2.0  |
| 32  | BK    | 42   | THR  | 2.0  |
| 36  | BO    | 77   | ALA  | 2.0  |
| 40  | BS    | 3    | THR  | 2.0  |
| 42  | BU    | 17   | ASP  | 2.0  |
| 43  | BW    | 46   | ALA  | 2.0  |
| 46  | DZ    | 14   | ALA  | 2.0  |
| 50  | B3    | 53   | ASP  | 2.0  |
| 52  | BI    | 113  | ALA  | 2.0  |
| 25  | DC    | 236  | GLY  | 2.0  |
| 32  | DK    | 96   | GLY  | 2.0  |
| 36  | DO    | 116  | GLN  | 2.0  |
| 42  | DU    | 89   | GLY  | 2.0  |
| 1   | AA    | 48   | C    | 2.0  |
| 1   | AA    | 322  | C    | 2.0  |
| 1   | AA    | 355  | C    | 2.0  |
| 1   | AA    | 400  | C    | 2.0  |
| 1   | CA    | 513  | C    | 2.0  |
| 8   | CI    | 114  | LYS  | 2.0  |
| 16  | AQ    | 48   | GLU  | 2.0  |
| 19  | AT    | 34   | VAL  | 2.0  |
| 23  | BB    | 985  | C    | 2.0  |
| 23  | BB    | 1208 | C    | 2.0  |
| 23  | DB    | 1790 | C    | 2.0  |
| 25  | BC    | 70   | LYS  | 2.0  |
| 29  | BG    | 172  | GLU  | 2.0  |
| 37  | DP    | 93   | LYS  | 2.0  |
| 26  | DD    | 73   | VAL  | 2.0  |
| 37  | BP    | 16   | VAL  | 2.0  |
| 39  | DR    | 54   | VAL  | 2.0  |
| 48  | B1    | 11   | VAL  | 2.0  |
| 1   | AA    | 198  | G    | 2.0  |
| 1   | AA    | 474  | G    | 2.0  |
| 1   | AA    | 803  | G    | 2.0  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | CA    | 785  | G    | 2.0  |
| 1   | CA    | 869  | G    | 2.0  |
| 2   | CC    | 125  | ARG  | 2.0  |
| 4   | AE    | 28   | ARG  | 2.0  |
| 6   | CG    | 91   | ARG  | 2.0  |
| 7   | AH    | 60   | LEU  | 2.0  |
| 7   | AH    | 98   | LEU  | 2.0  |
| 10  | AK    | 92   | ARG  | 2.0  |
| 14  | AO    | 66   | LEU  | 2.0  |
| 22  | DA    | 116  | G    | 2.0  |
| 23  | BB    | 1212 | G    | 2.0  |
| 23  | BB    | 1756 | G    | 2.0  |
| 23  | BB    | 2718 | G    | 2.0  |
| 23  | BB    | 2744 | G    | 2.0  |
| 23  | DB    | 978  | G    | 2.0  |
| 23  | DB    | 1062 | G    | 2.0  |
| 23  | DB    | 1935 | G    | 2.0  |
| 31  | DJ    | 114  | LEU  | 2.0  |
| 35  | BN    | 38   | LEU  | 2.0  |
| 44  | BX    | 28   | LEU  | 2.0  |
| 45  | DY    | 16   | LEU  | 2.0  |
| 19  | AT    | 56   | ILE  | 2.0  |
| 43  | BW    | 34   | SER  | 2.0  |
| 1   | AA    | 224  | U    | 2.0  |
| 1   | CA    | 850  | U    | 2.0  |
| 4   | CE    | 69   | ASN  | 2.0  |
| 22  | BA    | 25   | U    | 2.0  |
| 23  | BB    | 1629 | U    | 2.0  |
| 23  | BB    | 2016 | U    | 2.0  |
| 23  | BB    | 2796 | U    | 2.0  |
| 23  | DB    | 606  | U    | 2.0  |
| 23  | DB    | 931  | U    | 2.0  |
| 31  | DJ    | 128  | ASN  | 2.0  |
| 3   | AD    | 40   | HIS  | 2.0  |
| 3   | CD    | 169  | TRP  | 2.0  |
| 3   | CD    | 197  | HIS  | 2.0  |
| 26  | BD    | 67   | HIS  | 2.0  |
| 36  | BO    | 100  | HIS  | 2.0  |
| 12  | AM    | 54   | THR  | 2.0  |
| 20  | AB    | 215  | ALA  | 2.0  |
| 20  | CB    | 60   | ALA  | 2.0  |
| 29  | DG    | 33   | THR  | 2.0  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 30  | DH    | 69   | ALA  | 2.0  |
| 42  | BU    | 79   | ALA  | 2.0  |
| 40  | DS    | 38   | TYR  | 2.0  |
| 9   | CJ    | 63   | ASP  | 2.0  |
| 47  | B0    | 45   | ASP  | 2.0  |
| 12  | AM    | 62   | PHE  | 2.0  |
| 13  | AN    | 72   | PHE  | 2.0  |
| 14  | AO    | 15   | GLY  | 2.0  |
| 18  | CS    | 67   | GLY  | 2.0  |
| 26  | BD    | 166  | GLY  | 2.0  |
| 32  | BK    | 84   | CYS  | 2.0  |
| 34  | DM    | 83   | GLY  | 2.0  |
| 41  | BT    | 71   | GLY  | 2.0  |
| 42  | DU    | 56   | GLY  | 2.0  |
| 13  | AN    | 69   | PRO  | 2.0  |
| 14  | AO    | 61   | GLN  | 2.0  |
| 14  | CO    | 47   | LYS  | 2.0  |
| 14  | CO    | 72   | LYS  | 2.0  |
| 29  | BG    | 117  | PRO  | 2.0  |
| 30  | BH    | 83   | LYS  | 2.0  |
| 37  | DP    | 36   | LYS  | 2.0  |
| 51  | B4    | 31   | PRO  | 2.0  |
| 1   | AA    | 19   | A    | 2.0  |
| 1   | AA    | 878  | A    | 2.0  |
| 1   | AA    | 1287 | A    | 2.0  |
| 1   | CA    | 1375 | A    | 2.0  |
| 5   | CF    | 65   | GLU  | 2.0  |
| 6   | AG    | 86   | VAL  | 2.0  |
| 7   | CH    | 57   | GLU  | 2.0  |
| 11  | AL    | 51   | VAL  | 2.0  |
| 15  | CP    | 47   | GLU  | 2.0  |
| 18  | CS    | 72   | GLU  | 2.0  |
| 20  | CB    | 117  | GLU  | 2.0  |
| 23  | BB    | 643  | A    | 2.0  |
| 23  | BB    | 1634 | A    | 2.0  |
| 23  | BB    | 2721 | A    | 2.0  |
| 23  | DB    | 547  | A    | 2.0  |
| 23  | DB    | 1593 | A    | 2.0  |
| 23  | DB    | 1609 | A    | 2.0  |
| 23  | DB    | 2311 | A    | 2.0  |
| 25  | DC    | 22   | GLU  | 2.0  |
| 36  | DO    | 84   | GLU  | 2.0  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 26  | BD    | 184  | ARG  | 2.0  |
| 32  | DK    | 30   | ARG  | 2.0  |
| 33  | DL    | 116  | VAL  | 2.0  |
| 42  | BU    | 12   | VAL  | 2.0  |
| 43  | BW    | 28   | GLU  | 2.0  |
| 48  | D1    | 5    | ARG  | 2.0  |
| 5   | AF    | 54   | LEU  | 2.0  |
| 6   | CG    | 46   | LEU  | 2.0  |
| 7   | CH    | 10   | LEU  | 2.0  |
| 32  | DK    | 107  | LEU  | 2.0  |
| 35  | DN    | 54   | LEU  | 2.0  |
| 41  | DT    | 50   | LEU  | 2.0  |
| 52  | BI    | 48   | ILE  | 2.0  |
| 1   | AA    | 419  | C    | 2.0  |
| 1   | AA    | 1195 | C    | 2.0  |
| 1   | CA    | 1136 | C    | 2.0  |
| 23  | BB    | 961  | C    | 2.0  |
| 23  | BB    | 2691 | C    | 2.0  |
| 23  | DB    | 129  | C    | 2.0  |
| 23  | DB    | 440  | C    | 2.0  |
| 23  | DB    | 1178 | C    | 2.0  |
| 23  | DB    | 2755 | C    | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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 |
|-----|------|-------|------|-------|-------|------|----------------------------|-------|
| 54  | MG   | AA    | 1626 | 1/1   | -0.19 | 0.38 | 82,82,82,82                | 1     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC  | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|-----------------------------|-------|
| 54  | MG   | DB    | 3093 | 1/1   | -0.02 | 0.58 | 48,48,48,48                 | 1     |
| 54  | MG   | AA    | 1650 | 1/1   | 0.50  | 0.18 | 133,133,133,133             | 0     |
| 54  | MG   | CA    | 1624 | 1/1   | 0.61  | 0.15 | 162,162,162,162             | 0     |
| 54  | MG   | AA    | 1631 | 1/1   | 0.62  | 0.19 | 143,143,143,143             | 0     |
| 54  | MG   | DB    | 3058 | 1/1   | 0.63  | 0.15 | 132,132,132,132             | 0     |
| 54  | MG   | BB    | 3082 | 1/1   | 0.66  | 0.25 | 63,63,63,63                 | 0     |
| 54  | MG   | AA    | 1637 | 1/1   | 0.66  | 0.28 | 115,115,115,115             | 0     |
| 54  | MG   | CA    | 1616 | 1/1   | 0.67  | 0.17 | 153,153,153,153             | 0     |
| 53  | KSG  | AA    | 1601 | 26/26 | 0.74  | 0.21 | 53,53,53,53                 | 0     |
| 54  | MG   | AA    | 1639 | 1/1   | 0.78  | 0.17 | 141,141,141,141             | 0     |
| 54  | MG   | CA    | 1649 | 1/1   | 0.79  | 0.20 | 86,86,86,86                 | 0     |
| 54  | MG   | CA    | 1622 | 1/1   | 0.79  | 0.13 | 132,132,132,132             | 0     |
| 54  | MG   | BB    | 3100 | 1/1   | 0.79  | 0.26 | 37,37,37,37                 | 1     |
| 54  | MG   | CA    | 1629 | 1/1   | 0.80  | 0.14 | 62,62,62,62                 | 1     |
| 54  | MG   | DB    | 3064 | 1/1   | 0.80  | 0.42 | 66,66,66,66                 | 1     |
| 53  | KSG  | CA    | 1601 | 26/26 | 0.80  | 0.24 | 53,53,53,53                 | 0     |
| 54  | MG   | AA    | 1613 | 1/1   | 0.81  | 0.12 | 108,108,108,108             | 0     |
| 54  | MG   | BB    | 3041 | 1/1   | 0.81  | 0.12 | 47,47,47,47                 | 0     |
| 54  | MG   | AA    | 1620 | 1/1   | 0.81  | 0.09 | 116,116,116,116             | 0     |
| 54  | MG   | AA    | 1609 | 1/1   | 0.81  | 0.14 | 119,119,119,119             | 0     |
| 54  | MG   | AA    | 1615 | 1/1   | 0.82  | 0.14 | 72,72,72,72                 | 0     |
| 54  | MG   | AA    | 1621 | 1/1   | 0.82  | 0.11 | 96,96,96,96                 | 0     |
| 54  | MG   | AA    | 1628 | 1/1   | 0.84  | 0.14 | 63,63,63,63                 | 0     |
| 54  | MG   | CA    | 1640 | 1/1   | 0.84  | 0.09 | 139,139,139,139             | 0     |
| 54  | MG   | CA    | 1651 | 1/1   | 0.85  | 0.14 | 122,122,122,122             | 0     |
| 54  | MG   | BB    | 3047 | 1/1   | 0.85  | 0.24 | 128,128,128,128             | 0     |
| 54  | MG   | BB    | 3063 | 1/1   | 0.86  | 0.13 | 27,27,27,27                 | 0     |
| 54  | MG   | CA    | 1637 | 1/1   | 0.86  | 0.10 | 107,107,107,107             | 0     |
| 54  | MG   | AA    | 1647 | 1/1   | 0.86  | 0.22 | 84,84,84,84                 | 0     |
| 54  | MG   | BB    | 3028 | 1/1   | 0.86  | 0.21 | 66,66,66,66                 | 0     |
| 54  | MG   | DB    | 3013 | 1/1   | 0.87  | 0.12 | 32,32,32,32                 | 0     |
| 54  | MG   | DB    | 3033 | 1/1   | 0.87  | 0.19 | 88,88,88,88                 | 0     |
| 54  | MG   | AA    | 1616 | 1/1   | 0.87  | 0.08 | 86,86,86,86                 | 0     |
| 54  | MG   | BB    | 3067 | 1/1   | 0.87  | 0.12 | 56,56,56,56                 | 0     |
| 54  | MG   | BB    | 3034 | 1/1   | 0.87  | 0.13 | 42,42,42,42                 | 0     |
| 54  | MG   | CA    | 1609 | 1/1   | 0.88  | 0.17 | 132,132,132,132             | 0     |
| 54  | MG   | AA    | 1642 | 1/1   | 0.88  | 0.17 | 107,107,107,107             | 0     |
| 54  | MG   | AA    | 1652 | 1/1   | 0.88  | 0.14 | 105,105,105,105             | 0     |
| 54  | MG   | DB    | 3081 | 1/1   | 0.88  | 0.16 | 110,110,110,110             | 0     |
| 54  | MG   | CA    | 1638 | 1/1   | 0.88  | 0.10 | 60,60,60,60                 | 0     |
| 54  | MG   | DB    | 3106 | 1/1   | 0.88  | 0.07 | 7,7,7,7                     | 0     |
| 54  | MG   | CA    | 1628 | 1/1   | 0.89  | 0.13 | 38,38,38,38                 | 1     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BB    | 3008 | 1/1   | 0.89 | 0.12 | 82,82,82,82                 | 0     |
| 54  | MG   | BB    | 3107 | 1/1   | 0.89 | 0.10 | 37,37,37,37                 | 0     |
| 54  | MG   | DB    | 3059 | 1/1   | 0.89 | 0.11 | 75,75,75,75                 | 0     |
| 54  | MG   | BB    | 3060 | 1/1   | 0.89 | 0.13 | 81,81,81,81                 | 0     |
| 54  | MG   | AA    | 1625 | 1/1   | 0.89 | 0.15 | 81,81,81,81                 | 0     |
| 54  | MG   | AA    | 1603 | 1/1   | 0.89 | 0.09 | 74,74,74,74                 | 0     |
| 54  | MG   | AA    | 1633 | 1/1   | 0.89 | 0.11 | 92,92,92,92                 | 0     |
| 54  | MG   | BB    | 3018 | 1/1   | 0.90 | 0.12 | 42,42,42,42                 | 0     |
| 54  | MG   | BB    | 3007 | 1/1   | 0.90 | 0.10 | 57,57,57,57                 | 0     |
| 54  | MG   | AA    | 1659 | 1/1   | 0.90 | 0.19 | 157,157,157,157             | 0     |
| 54  | MG   | DB    | 3060 | 1/1   | 0.91 | 0.11 | 105,105,105,105             | 0     |
| 54  | MG   | CA    | 1617 | 1/1   | 0.91 | 0.11 | 45,45,45,45                 | 0     |
| 54  | MG   | AA    | 1624 | 1/1   | 0.91 | 0.23 | 25,25,25,25                 | 1     |
| 54  | MG   | CA    | 1635 | 1/1   | 0.91 | 0.15 | 91,91,91,91                 | 0     |
| 54  | MG   | AA    | 1649 | 1/1   | 0.91 | 0.09 | 102,102,102,102             | 0     |
| 54  | MG   | AA    | 1608 | 1/1   | 0.92 | 0.14 | 57,57,57,57                 | 0     |
| 54  | MG   | CA    | 1627 | 1/1   | 0.92 | 0.17 | 114,114,114,114             | 0     |
| 54  | MG   | BB    | 3081 | 1/1   | 0.92 | 0.12 | 34,34,34,34                 | 0     |
| 54  | MG   | AA    | 1658 | 1/1   | 0.92 | 0.12 | 113,113,113,113             | 0     |
| 54  | MG   | AA    | 1623 | 1/1   | 0.92 | 0.09 | 143,143,143,143             | 0     |
| 54  | MG   | DB    | 3082 | 1/1   | 0.92 | 0.21 | 61,61,61,61                 | 0     |
| 54  | MG   | BB    | 3106 | 1/1   | 0.92 | 0.11 | 62,62,62,62                 | 0     |
| 54  | MG   | DB    | 3049 | 1/1   | 0.92 | 0.07 | 79,79,79,79                 | 0     |
| 54  | MG   | AA    | 1634 | 1/1   | 0.93 | 0.10 | 73,73,73,73                 | 0     |
| 54  | MG   | BB    | 3092 | 1/1   | 0.93 | 0.10 | 56,56,56,56                 | 0     |
| 54  | MG   | BB    | 3097 | 1/1   | 0.93 | 0.07 | 96,96,96,96                 | 0     |
| 54  | MG   | AA    | 1636 | 1/1   | 0.93 | 0.13 | 83,83,83,83                 | 0     |
| 54  | MG   | AA    | 1627 | 1/1   | 0.93 | 0.13 | 17,17,17,17                 | 1     |
| 54  | MG   | AA    | 1618 | 1/1   | 0.93 | 0.10 | 102,102,102,102             | 0     |
| 54  | MG   | AA    | 1640 | 1/1   | 0.93 | 0.08 | 42,42,42,42                 | 0     |
| 54  | MG   | DB    | 3075 | 1/1   | 0.93 | 0.09 | 42,42,42,42                 | 0     |
| 54  | MG   | AA    | 1654 | 1/1   | 0.93 | 0.08 | 81,81,81,81                 | 0     |
| 54  | MG   | BB    | 3072 | 1/1   | 0.93 | 0.09 | 26,26,26,26                 | 0     |
| 54  | MG   | BB    | 3033 | 1/1   | 0.93 | 0.12 | 113,113,113,113             | 0     |
| 54  | MG   | CA    | 1661 | 1/1   | 0.93 | 0.10 | 67,67,67,67                 | 0     |
| 54  | MG   | DE    | 301  | 1/1   | 0.93 | 0.10 | 69,69,69,69                 | 0     |
| 54  | MG   | BB    | 3109 | 1/1   | 0.94 | 0.09 | 33,33,33,33                 | 0     |
| 54  | MG   | CA    | 1607 | 1/1   | 0.94 | 0.11 | 126,126,126,126             | 0     |
| 54  | MG   | BB    | 3089 | 1/1   | 0.94 | 0.12 | 82,82,82,82                 | 0     |
| 54  | MG   | CA    | 1612 | 1/1   | 0.94 | 0.07 | 71,71,71,71                 | 0     |
| 54  | MG   | AA    | 1657 | 1/1   | 0.94 | 0.12 | 83,83,83,83                 | 0     |
| 54  | MG   | BB    | 3073 | 1/1   | 0.94 | 0.10 | 55,55,55,55                 | 0     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DB    | 3076 | 1/1   | 0.94 | 0.10 | 69,69,69,69                 | 0     |
| 54  | MG   | BB    | 3099 | 1/1   | 0.94 | 0.10 | 58,58,58,58                 | 0     |
| 54  | MG   | BB    | 3064 | 1/1   | 0.94 | 0.10 | 71,71,71,71                 | 0     |
| 54  | MG   | AA    | 1602 | 1/1   | 0.94 | 0.09 | 34,34,34,34                 | 0     |
| 54  | MG   | DB    | 3015 | 1/1   | 0.94 | 0.12 | 69,69,69,69                 | 0     |
| 54  | MG   | DB    | 3108 | 1/1   | 0.94 | 0.08 | 24,24,24,24                 | 0     |
| 54  | MG   | BB    | 3087 | 1/1   | 0.94 | 0.08 | 53,53,53,53                 | 0     |
| 54  | MG   | AA    | 1656 | 1/1   | 0.95 | 0.07 | 100,100,100,100             | 0     |
| 54  | MG   | DB    | 3034 | 1/1   | 0.95 | 0.09 | 84,84,84,84                 | 0     |
| 54  | MG   | AA    | 1660 | 1/1   | 0.95 | 0.09 | 95,95,95,95                 | 0     |
| 54  | MG   | DB    | 3052 | 1/1   | 0.95 | 0.16 | 42,42,42,42                 | 0     |
| 54  | MG   | BB    | 3091 | 1/1   | 0.95 | 0.08 | 42,42,42,42                 | 0     |
| 54  | MG   | AA    | 1646 | 1/1   | 0.95 | 0.10 | 103,103,103,103             | 0     |
| 54  | MG   | CA    | 1614 | 1/1   | 0.95 | 0.07 | 97,97,97,97                 | 0     |
| 54  | MG   | AA    | 1655 | 1/1   | 0.95 | 0.08 | 67,67,67,67                 | 0     |
| 54  | MG   | CA    | 1644 | 1/1   | 0.95 | 0.09 | 59,59,59,59                 | 0     |
| 54  | MG   | BB    | 3010 | 1/1   | 0.95 | 0.15 | 74,74,74,74                 | 0     |
| 54  | MG   | BB    | 3042 | 1/1   | 0.95 | 0.06 | 74,74,74,74                 | 0     |
| 54  | MG   | CA    | 1659 | 1/1   | 0.95 | 0.10 | 88,88,88,88                 | 0     |
| 54  | MG   | DB    | 3088 | 1/1   | 0.95 | 0.08 | 51,51,51,51                 | 0     |
| 54  | MG   | CA    | 1623 | 1/1   | 0.95 | 0.07 | 77,77,77,77                 | 0     |
| 54  | MG   | BB    | 3012 | 1/1   | 0.95 | 0.09 | 75,75,75,75                 | 0     |
| 54  | MG   | BB    | 3048 | 1/1   | 0.95 | 0.08 | 39,39,39,39                 | 0     |
| 54  | MG   | DB    | 3029 | 1/1   | 0.95 | 0.10 | 22,22,22,22                 | 0     |
| 54  | MG   | DB    | 3027 | 1/1   | 0.96 | 0.07 | 37,37,37,37                 | 0     |
| 54  | MG   | BB    | 3105 | 1/1   | 0.96 | 0.11 | 33,33,33,33                 | 0     |
| 54  | MG   | BB    | 3051 | 1/1   | 0.96 | 0.06 | 74,74,74,74                 | 0     |
| 54  | MG   | BB    | 3056 | 1/1   | 0.96 | 0.09 | 37,37,37,37                 | 0     |
| 54  | MG   | DB    | 3035 | 1/1   | 0.96 | 0.08 | 24,24,24,24                 | 0     |
| 54  | MG   | DB    | 3040 | 1/1   | 0.96 | 0.10 | 28,28,28,28                 | 0     |
| 54  | MG   | CA    | 1631 | 1/1   | 0.96 | 0.07 | 21,21,21,21                 | 1     |
| 54  | MG   | BB    | 3086 | 1/1   | 0.96 | 0.20 | 94,94,94,94                 | 0     |
| 54  | MG   | BB    | 3110 | 1/1   | 0.96 | 0.19 | 79,79,79,79                 | 0     |
| 54  | MG   | AA    | 1645 | 1/1   | 0.96 | 0.07 | 97,97,97,97                 | 0     |
| 54  | MG   | AA    | 1661 | 1/1   | 0.96 | 0.10 | 83,83,83,83                 | 0     |
| 54  | MG   | DB    | 3061 | 1/1   | 0.96 | 0.08 | 48,48,48,48                 | 0     |
| 54  | MG   | CA    | 1642 | 1/1   | 0.96 | 0.10 | 70,70,70,70                 | 0     |
| 54  | MG   | DB    | 3071 | 1/1   | 0.96 | 0.08 | 27,27,27,27                 | 0     |
| 54  | MG   | BB    | 3005 | 1/1   | 0.96 | 0.15 | 13,13,13,13                 | 0     |
| 54  | MG   | CA    | 1646 | 1/1   | 0.96 | 0.07 | 94,94,94,94                 | 0     |
| 54  | MG   | DB    | 3080 | 1/1   | 0.96 | 0.08 | 34,34,34,34                 | 0     |
| 54  | MG   | BB    | 3043 | 1/1   | 0.96 | 0.10 | 63,63,63,63                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | AA    | 1617 | 1/1   | 0.96 | 0.09 | 65,65,65,65                 | 0     |
| 54  | MG   | DB    | 3083 | 1/1   | 0.96 | 0.07 | 18,18,18,18                 | 0     |
| 54  | MG   | BB    | 3098 | 1/1   | 0.96 | 0.12 | 49,49,49,49                 | 0     |
| 54  | MG   | DB    | 3090 | 1/1   | 0.96 | 0.08 | 106,106,106,106             | 0     |
| 54  | MG   | AA    | 1614 | 1/1   | 0.96 | 0.07 | 67,67,67,67                 | 0     |
| 54  | MG   | DB    | 3094 | 1/1   | 0.96 | 0.14 | 33,33,33,33                 | 0     |
| 54  | MG   | DB    | 3102 | 1/1   | 0.96 | 0.09 | 13,13,13,13                 | 0     |
| 54  | MG   | DB    | 3103 | 1/1   | 0.96 | 0.12 | 61,61,61,61                 | 0     |
| 54  | MG   | BB    | 3077 | 1/1   | 0.96 | 0.09 | 37,37,37,37                 | 0     |
| 54  | MG   | BB    | 3102 | 1/1   | 0.96 | 0.06 | 34,34,34,34                 | 0     |
| 54  | MG   | DB    | 3020 | 1/1   | 0.96 | 0.13 | 41,41,41,41                 | 0     |
| 54  | MG   | DN    | 201  | 1/1   | 0.96 | 0.10 | 38,38,38,38                 | 0     |
| 54  | MG   | DB    | 3024 | 1/1   | 0.97 | 0.06 | 27,27,27,27                 | 0     |
| 54  | MG   | BB    | 3078 | 1/1   | 0.97 | 0.14 | 49,49,49,49                 | 0     |
| 54  | MG   | BB    | 3014 | 1/1   | 0.97 | 0.07 | 33,33,33,33                 | 0     |
| 54  | MG   | BB    | 3046 | 1/1   | 0.97 | 0.09 | 63,63,63,63                 | 0     |
| 54  | MG   | BB    | 3017 | 1/1   | 0.97 | 0.09 | 54,54,54,54                 | 0     |
| 54  | MG   | CA    | 1621 | 1/1   | 0.97 | 0.07 | 46,46,46,46                 | 0     |
| 54  | MG   | AA    | 1622 | 1/1   | 0.97 | 0.03 | 16,16,16,16                 | 0     |
| 54  | MG   | DB    | 3044 | 1/1   | 0.97 | 0.07 | 58,58,58,58                 | 0     |
| 54  | MG   | BB    | 3019 | 1/1   | 0.97 | 0.10 | 22,22,22,22                 | 0     |
| 54  | MG   | DB    | 3050 | 1/1   | 0.97 | 0.10 | 42,42,42,42                 | 0     |
| 54  | MG   | BB    | 3090 | 1/1   | 0.97 | 0.06 | 65,65,65,65                 | 0     |
| 54  | MG   | DB    | 3057 | 1/1   | 0.97 | 0.18 | 56,56,56,56                 | 1     |
| 54  | MG   | BB    | 3053 | 1/1   | 0.97 | 0.06 | 36,36,36,36                 | 0     |
| 54  | MG   | BB    | 3021 | 1/1   | 0.97 | 0.10 | 24,24,24,24                 | 0     |
| 54  | MG   | BB    | 3096 | 1/1   | 0.97 | 0.05 | 39,39,39,39                 | 0     |
| 54  | MG   | CA    | 1630 | 1/1   | 0.97 | 0.06 | 49,49,49,49                 | 0     |
| 54  | MG   | DB    | 3062 | 1/1   | 0.97 | 0.09 | 24,24,24,24                 | 0     |
| 54  | MG   | AA    | 1619 | 1/1   | 0.97 | 0.05 | 33,33,33,33                 | 0     |
| 54  | MG   | DB    | 3069 | 1/1   | 0.97 | 0.05 | 50,50,50,50                 | 0     |
| 54  | MG   | BB    | 3062 | 1/1   | 0.97 | 0.11 | 34,34,34,34                 | 0     |
| 54  | MG   | DB    | 3073 | 1/1   | 0.97 | 0.06 | 44,44,44,44                 | 0     |
| 54  | MG   | BB    | 3030 | 1/1   | 0.97 | 0.06 | 45,45,45,45                 | 0     |
| 54  | MG   | BB    | 3031 | 1/1   | 0.97 | 0.08 | 46,46,46,46                 | 0     |
| 54  | MG   | BB    | 3065 | 1/1   | 0.97 | 0.08 | 47,47,47,47                 | 0     |
| 54  | MG   | BB    | 3104 | 1/1   | 0.97 | 0.07 | 33,33,33,33                 | 0     |
| 54  | MG   | BB    | 3066 | 1/1   | 0.97 | 0.07 | 42,42,42,42                 | 0     |
| 54  | MG   | AA    | 1604 | 1/1   | 0.97 | 0.07 | 25,25,25,25                 | 0     |
| 54  | MG   | CA    | 1648 | 1/1   | 0.97 | 0.06 | 39,39,39,39                 | 0     |
| 54  | MG   | BB    | 3071 | 1/1   | 0.97 | 0.09 | 38,38,38,38                 | 0     |
| 54  | MG   | BB    | 3108 | 1/1   | 0.97 | 0.07 | 22,22,22,22                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | AA    | 1643 | 1/1   | 0.97 | 0.06 | 116,116,116,116             | 0     |
| 54  | MG   | AA    | 1644 | 1/1   | 0.97 | 0.11 | 81,81,81,81                 | 0     |
| 54  | MG   | CA    | 1604 | 1/1   | 0.97 | 0.12 | 49,49,49,49                 | 0     |
| 54  | MG   | BB    | 3076 | 1/1   | 0.97 | 0.06 | 43,43,43,43                 | 0     |
| 54  | MG   | DB    | 3107 | 1/1   | 0.97 | 0.09 | 19,19,19,19                 | 0     |
| 54  | MG   | DB    | 3016 | 1/1   | 0.97 | 0.08 | 25,25,25,25                 | 0     |
| 54  | MG   | AA    | 1607 | 1/1   | 0.97 | 0.06 | 82,82,82,82                 | 0     |
| 54  | MG   | DB    | 3023 | 1/1   | 0.97 | 0.06 | 44,44,44,44                 | 0     |
| 54  | MG   | BB    | 3068 | 1/1   | 0.98 | 0.07 | 39,39,39,39                 | 0     |
| 54  | MG   | DB    | 3014 | 1/1   | 0.98 | 0.06 | 28,28,28,28                 | 0     |
| 54  | MG   | BB    | 3036 | 1/1   | 0.98 | 0.06 | 29,29,29,29                 | 0     |
| 54  | MG   | BB    | 3038 | 1/1   | 0.98 | 0.03 | 82,82,82,82                 | 0     |
| 54  | MG   | DB    | 3018 | 1/1   | 0.98 | 0.06 | 39,39,39,39                 | 0     |
| 54  | MG   | BB    | 3039 | 1/1   | 0.98 | 0.07 | 26,26,26,26                 | 0     |
| 54  | MG   | BB    | 3075 | 1/1   | 0.98 | 0.17 | 35,35,35,35                 | 0     |
| 54  | MG   | BB    | 3013 | 1/1   | 0.98 | 0.07 | 36,36,36,36                 | 0     |
| 54  | MG   | AA    | 1605 | 1/1   | 0.98 | 0.08 | 30,30,30,30                 | 0     |
| 54  | MG   | DB    | 3028 | 1/1   | 0.98 | 0.09 | 29,29,29,29                 | 0     |
| 54  | MG   | BB    | 3016 | 1/1   | 0.98 | 0.12 | 19,19,19,19                 | 0     |
| 54  | MG   | CA    | 1613 | 1/1   | 0.98 | 0.08 | 63,63,63,63                 | 0     |
| 54  | MG   | BB    | 3079 | 1/1   | 0.98 | 0.05 | 32,32,32,32                 | 0     |
| 54  | MG   | BB    | 3080 | 1/1   | 0.98 | 0.05 | 42,42,42,42                 | 0     |
| 54  | MG   | AA    | 1641 | 1/1   | 0.98 | 0.04 | 72,72,72,72                 | 0     |
| 54  | MG   | AA    | 1611 | 1/1   | 0.98 | 0.05 | 57,57,57,57                 | 0     |
| 54  | MG   | DB    | 3046 | 1/1   | 0.98 | 0.11 | 18,18,18,18                 | 0     |
| 54  | MG   | DB    | 3047 | 1/1   | 0.98 | 0.06 | 29,29,29,29                 | 0     |
| 54  | MG   | BB    | 3083 | 1/1   | 0.98 | 0.07 | 25,25,25,25                 | 0     |
| 54  | MG   | BB    | 3084 | 1/1   | 0.98 | 0.06 | 19,19,19,19                 | 0     |
| 54  | MG   | DB    | 3051 | 1/1   | 0.98 | 0.09 | 57,57,57,57                 | 0     |
| 54  | MG   | BB    | 3001 | 1/1   | 0.98 | 0.06 | 28,28,28,28                 | 0     |
| 54  | MG   | DB    | 3053 | 1/1   | 0.98 | 0.06 | 37,37,37,37                 | 0     |
| 54  | MG   | DB    | 3056 | 1/1   | 0.98 | 0.10 | 67,67,67,67                 | 0     |
| 54  | MG   | BB    | 3004 | 1/1   | 0.98 | 0.05 | 39,39,39,39                 | 0     |
| 54  | MG   | BB    | 3088 | 1/1   | 0.98 | 0.11 | 25,25,25,25                 | 0     |
| 54  | MG   | BB    | 3052 | 1/1   | 0.98 | 0.05 | 27,27,27,27                 | 0     |
| 54  | MG   | BB    | 3022 | 1/1   | 0.98 | 0.06 | 55,55,55,55                 | 0     |
| 54  | MG   | BB    | 3054 | 1/1   | 0.98 | 0.10 | 77,77,77,77                 | 0     |
| 54  | MG   | CA    | 1632 | 1/1   | 0.98 | 0.07 | 34,34,34,34                 | 0     |
| 54  | MG   | CA    | 1634 | 1/1   | 0.98 | 0.07 | 46,46,46,46                 | 0     |
| 54  | MG   | DB    | 3068 | 1/1   | 0.98 | 0.05 | 49,49,49,49                 | 0     |
| 54  | MG   | BB    | 3055 | 1/1   | 0.98 | 0.08 | 19,19,19,19                 | 0     |
| 54  | MG   | BB    | 3094 | 1/1   | 0.98 | 0.08 | 16,16,16,16                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BB    | 3023 | 1/1   | 0.98 | 0.07 | 27,27,27,27                 | 0     |
| 54  | MG   | BB    | 3058 | 1/1   | 0.98 | 0.05 | 33,33,33,33                 | 0     |
| 54  | MG   | BB    | 3024 | 1/1   | 0.98 | 0.09 | 22,22,22,22                 | 0     |
| 54  | MG   | CA    | 1643 | 1/1   | 0.98 | 0.07 | 62,62,62,62                 | 0     |
| 54  | MG   | BB    | 3026 | 1/1   | 0.98 | 0.05 | 25,25,25,25                 | 0     |
| 54  | MG   | AA    | 1635 | 1/1   | 0.98 | 0.04 | 75,75,75,75                 | 0     |
| 54  | MG   | CA    | 1647 | 1/1   | 0.98 | 0.08 | 40,40,40,40                 | 0     |
| 54  | MG   | DB    | 3085 | 1/1   | 0.98 | 0.12 | 64,64,64,64                 | 0     |
| 54  | MG   | DB    | 3087 | 1/1   | 0.98 | 0.09 | 40,40,40,40                 | 0     |
| 54  | MG   | BB    | 3101 | 1/1   | 0.98 | 0.06 | 14,14,14,14                 | 0     |
| 54  | MG   | AA    | 1612 | 1/1   | 0.98 | 0.07 | 52,52,52,52                 | 0     |
| 54  | MG   | DB    | 3091 | 1/1   | 0.98 | 0.08 | 39,39,39,39                 | 0     |
| 54  | MG   | CA    | 1650 | 1/1   | 0.98 | 0.09 | 67,67,67,67                 | 0     |
| 54  | MG   | AA    | 1629 | 1/1   | 0.98 | 0.11 | 62,62,62,62                 | 0     |
| 54  | MG   | DB    | 3095 | 1/1   | 0.98 | 0.07 | 44,44,44,44                 | 0     |
| 54  | MG   | DB    | 3099 | 1/1   | 0.98 | 0.07 | 11,11,11,11                 | 0     |
| 54  | MG   | DB    | 3101 | 1/1   | 0.98 | 0.04 | 30,30,30,30                 | 0     |
| 54  | MG   | CA    | 1657 | 1/1   | 0.98 | 0.10 | 51,51,51,51                 | 0     |
| 54  | MG   | AA    | 1638 | 1/1   | 0.98 | 0.11 | 88,88,88,88                 | 0     |
| 54  | MG   | DB    | 3104 | 1/1   | 0.98 | 0.10 | 44,44,44,44                 | 0     |
| 54  | MG   | CA    | 1660 | 1/1   | 0.98 | 0.12 | 27,27,27,27                 | 0     |
| 54  | MG   | AA    | 1606 | 1/1   | 0.98 | 0.05 | 28,28,28,28                 | 0     |
| 54  | MG   | CA    | 1663 | 1/1   | 0.98 | 0.07 | 20,20,20,20                 | 0     |
| 54  | MG   | DB    | 3109 | 1/1   | 0.98 | 0.10 | 57,57,57,57                 | 0     |
| 54  | MG   | DB    | 3002 | 1/1   | 0.98 | 0.06 | 20,20,20,20                 | 0     |
| 54  | MG   | DB    | 3007 | 1/1   | 0.98 | 0.06 | 15,15,15,15                 | 0     |
| 54  | MG   | AA    | 1632 | 1/1   | 0.99 | 0.07 | 44,44,44,44                 | 0     |
| 54  | MG   | DB    | 3025 | 1/1   | 0.99 | 0.15 | 20,20,20,20                 | 0     |
| 54  | MG   | DB    | 3026 | 1/1   | 0.99 | 0.11 | 30,30,30,30                 | 0     |
| 54  | MG   | BB    | 3049 | 1/1   | 0.99 | 0.05 | 12,12,12,12                 | 0     |
| 54  | MG   | BB    | 3050 | 1/1   | 0.99 | 0.03 | 20,20,20,20                 | 0     |
| 54  | MG   | BB    | 3006 | 1/1   | 0.99 | 0.05 | 20,20,20,20                 | 0     |
| 54  | MG   | DB    | 3031 | 1/1   | 0.99 | 0.04 | 40,40,40,40                 | 0     |
| 54  | MG   | DB    | 3032 | 1/1   | 0.99 | 0.08 | 29,29,29,29                 | 0     |
| 54  | MG   | BB    | 3032 | 1/1   | 0.99 | 0.04 | 31,31,31,31                 | 0     |
| 54  | MG   | AA    | 1630 | 1/1   | 0.99 | 0.04 | 20,20,20,20                 | 0     |
| 54  | MG   | CA    | 1633 | 1/1   | 0.99 | 0.03 | 50,50,50,50                 | 0     |
| 54  | MG   | DB    | 3036 | 1/1   | 0.99 | 0.09 | 25,25,25,25                 | 0     |
| 54  | MG   | DB    | 3038 | 1/1   | 0.99 | 0.04 | 33,33,33,33                 | 0     |
| 54  | MG   | AA    | 1651 | 1/1   | 0.99 | 0.05 | 64,64,64,64                 | 0     |
| 54  | MG   | DB    | 3042 | 1/1   | 0.99 | 0.05 | 5,5,5,5                     | 0     |
| 54  | MG   | BB    | 3009 | 1/1   | 0.99 | 0.04 | 35,35,35,35                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DB    | 3045 | 1/1   | 0.99 | 0.04 | 45,45,45,45                 | 0     |
| 54  | MG   | CA    | 1636 | 1/1   | 0.99 | 0.08 | 13,13,13,13                 | 0     |
| 54  | MG   | AA    | 1648 | 1/1   | 0.99 | 0.08 | 31,31,31,31                 | 0     |
| 54  | MG   | BB    | 3057 | 1/1   | 0.99 | 0.10 | 19,19,19,19                 | 0     |
| 54  | MG   | CA    | 1639 | 1/1   | 0.99 | 0.04 | 41,41,41,41                 | 0     |
| 54  | MG   | BB    | 3002 | 1/1   | 0.99 | 0.05 | 9,9,9,9                     | 0     |
| 54  | MG   | CA    | 1641 | 1/1   | 0.99 | 0.07 | 40,40,40,40                 | 0     |
| 54  | MG   | BB    | 3040 | 1/1   | 0.99 | 0.07 | 18,18,18,18                 | 0     |
| 54  | MG   | DB    | 3054 | 1/1   | 0.99 | 0.05 | 32,32,32,32                 | 0     |
| 54  | MG   | BB    | 3061 | 1/1   | 0.99 | 0.04 | 33,33,33,33                 | 0     |
| 54  | MG   | CA    | 1603 | 1/1   | 0.99 | 0.10 | 32,32,32,32                 | 0     |
| 54  | MG   | CA    | 1645 | 1/1   | 0.99 | 0.05 | 28,28,28,28                 | 0     |
| 54  | MG   | BB    | 3085 | 1/1   | 0.99 | 0.06 | 67,67,67,67                 | 0     |
| 54  | MG   | CA    | 1605 | 1/1   | 0.99 | 0.05 | 37,37,37,37                 | 0     |
| 54  | MG   | CA    | 1606 | 1/1   | 0.99 | 0.08 | 30,30,30,30                 | 0     |
| 54  | MG   | BB    | 3003 | 1/1   | 0.99 | 0.04 | 23,23,23,23                 | 0     |
| 54  | MG   | CA    | 1608 | 1/1   | 0.99 | 0.04 | 31,31,31,31                 | 0     |
| 54  | MG   | DB    | 3065 | 1/1   | 0.99 | 0.06 | 25,25,25,25                 | 0     |
| 54  | MG   | DB    | 3066 | 1/1   | 0.99 | 0.05 | 12,12,12,12                 | 0     |
| 54  | MG   | DB    | 3067 | 1/1   | 0.99 | 0.17 | 11,11,11,11                 | 0     |
| 54  | MG   | BB    | 3025 | 1/1   | 0.99 | 0.12 | 67,67,67,67                 | 0     |
| 54  | MG   | CA    | 1652 | 1/1   | 0.99 | 0.10 | 20,20,20,20                 | 0     |
| 54  | MG   | DB    | 3070 | 1/1   | 0.99 | 0.04 | 60,60,60,60                 | 0     |
| 54  | MG   | CA    | 1653 | 1/1   | 0.99 | 0.03 | 48,48,48,48                 | 0     |
| 54  | MG   | CA    | 1654 | 1/1   | 0.99 | 0.10 | 32,32,32,32                 | 0     |
| 54  | MG   | CA    | 1655 | 1/1   | 0.99 | 0.05 | 26,26,26,26                 | 0     |
| 54  | MG   | CA    | 1656 | 1/1   | 0.99 | 0.03 | 60,60,60,60                 | 0     |
| 54  | MG   | DB    | 3077 | 1/1   | 0.99 | 0.05 | 41,41,41,41                 | 0     |
| 54  | MG   | CA    | 1610 | 1/1   | 0.99 | 0.04 | 61,61,61,61                 | 0     |
| 54  | MG   | CA    | 1658 | 1/1   | 0.99 | 0.04 | 18,18,18,18                 | 0     |
| 54  | MG   | AA    | 1653 | 1/1   | 0.99 | 0.06 | 30,30,30,30                 | 0     |
| 54  | MG   | BB    | 3044 | 1/1   | 0.99 | 0.04 | 39,39,39,39                 | 0     |
| 54  | MG   | BB    | 3045 | 1/1   | 0.99 | 0.03 | 40,40,40,40                 | 0     |
| 54  | MG   | DB    | 3086 | 1/1   | 0.99 | 0.10 | 25,25,25,25                 | 0     |
| 54  | MG   | CA    | 1662 | 1/1   | 0.99 | 0.03 | 38,38,38,38                 | 0     |
| 54  | MG   | CA    | 1615 | 1/1   | 0.99 | 0.06 | 54,54,54,54                 | 0     |
| 54  | MG   | DB    | 3089 | 1/1   | 0.99 | 0.14 | 28,28,28,28                 | 0     |
| 54  | MG   | DB    | 3001 | 1/1   | 0.99 | 0.08 | 5,5,5,5                     | 0     |
| 54  | MG   | BB    | 3027 | 1/1   | 0.99 | 0.04 | 29,29,29,29                 | 0     |
| 54  | MG   | DB    | 3092 | 1/1   | 0.99 | 0.03 | 16,16,16,16                 | 0     |
| 54  | MG   | DB    | 3003 | 1/1   | 0.99 | 0.06 | 8,8,8,8                     | 0     |
| 54  | MG   | DB    | 3004 | 1/1   | 0.99 | 0.12 | 38,38,38,38                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BB    | 3015 | 1/1   | 0.99 | 0.04 | 23,23,23,23                 | 0     |
| 54  | MG   | DB    | 3097 | 1/1   | 0.99 | 0.08 | 19,19,19,19                 | 0     |
| 54  | MG   | DB    | 3098 | 1/1   | 0.99 | 0.05 | 9,9,9,9                     | 0     |
| 54  | MG   | DB    | 3009 | 1/1   | 0.99 | 0.03 | 10,10,10,10                 | 0     |
| 54  | MG   | DB    | 3100 | 1/1   | 0.99 | 0.07 | 6,6,6,6                     | 0     |
| 54  | MG   | DB    | 3012 | 1/1   | 0.99 | 0.10 | 6,6,6,6                     | 0     |
| 54  | MG   | CA    | 1620 | 1/1   | 0.99 | 0.11 | 32,32,32,32                 | 0     |
| 54  | MG   | BB    | 3093 | 1/1   | 0.99 | 0.16 | 5,5,5,5                     | 1     |
| 54  | MG   | BB    | 3069 | 1/1   | 0.99 | 0.04 | 8,8,8,8                     | 0     |
| 54  | MG   | DB    | 3105 | 1/1   | 0.99 | 0.05 | 24,24,24,24                 | 0     |
| 54  | MG   | BB    | 3095 | 1/1   | 0.99 | 0.04 | 48,48,48,48                 | 0     |
| 54  | MG   | DB    | 3017 | 1/1   | 0.99 | 0.10 | 22,22,22,22                 | 0     |
| 54  | MG   | BB    | 3070 | 1/1   | 0.99 | 0.07 | 55,55,55,55                 | 0     |
| 54  | MG   | CA    | 1625 | 1/1   | 0.99 | 0.04 | 24,24,24,24                 | 0     |
| 54  | MG   | DB    | 3021 | 1/1   | 0.99 | 0.06 | 25,25,25,25                 | 0     |
| 54  | MG   | CA    | 1626 | 1/1   | 0.99 | 0.05 | 17,17,17,17                 | 0     |
| 54  | MG   | DB    | 3078 | 1/1   | 1.00 | 0.02 | 5,5,5,5                     | 0     |
| 54  | MG   | DB    | 3079 | 1/1   | 1.00 | 0.03 | 7,7,7,7                     | 0     |
| 54  | MG   | DB    | 3048 | 1/1   | 1.00 | 0.02 | 7,7,7,7                     | 0     |
| 54  | MG   | BB    | 3011 | 1/1   | 1.00 | 0.05 | 9,9,9,9                     | 0     |
| 54  | MG   | BB    | 3103 | 1/1   | 1.00 | 0.07 | 11,11,11,11                 | 0     |
| 54  | MG   | DB    | 3005 | 1/1   | 1.00 | 0.03 | 6,6,6,6                     | 0     |
| 54  | MG   | DB    | 3084 | 1/1   | 1.00 | 0.03 | 18,18,18,18                 | 0     |
| 54  | MG   | DB    | 3006 | 1/1   | 1.00 | 0.02 | 16,16,16,16                 | 0     |
| 54  | MG   | BB    | 3029 | 1/1   | 1.00 | 0.02 | 7,7,7,7                     | 0     |
| 54  | MG   | DB    | 3008 | 1/1   | 1.00 | 0.10 | 39,39,39,39                 | 0     |
| 54  | MG   | DB    | 3055 | 1/1   | 1.00 | 0.08 | 20,20,20,20                 | 0     |
| 54  | MG   | BB    | 3020 | 1/1   | 1.00 | 0.03 | 38,38,38,38                 | 0     |
| 54  | MG   | DB    | 3030 | 1/1   | 1.00 | 0.06 | 11,11,11,11                 | 0     |
| 54  | MG   | DB    | 3010 | 1/1   | 1.00 | 0.03 | 8,8,8,8                     | 0     |
| 54  | MG   | DB    | 3011 | 1/1   | 1.00 | 0.09 | 23,23,23,23                 | 0     |
| 54  | MG   | CA    | 1618 | 1/1   | 1.00 | 0.04 | 26,26,26,26                 | 0     |
| 54  | MG   | CA    | 1619 | 1/1   | 1.00 | 0.03 | 9,9,9,9                     | 0     |
| 54  | MG   | BB    | 3059 | 1/1   | 1.00 | 0.03 | 16,16,16,16                 | 0     |
| 54  | MG   | DB    | 3096 | 1/1   | 1.00 | 0.10 | 31,31,31,31                 | 0     |
| 54  | MG   | DB    | 3063 | 1/1   | 1.00 | 0.03 | 42,42,42,42                 | 0     |
| 54  | MG   | BB    | 3074 | 1/1   | 1.00 | 0.05 | 7,7,7,7                     | 0     |
| 54  | MG   | DB    | 3037 | 1/1   | 1.00 | 0.02 | 8,8,8,8                     | 0     |
| 54  | MG   | BB    | 3035 | 1/1   | 1.00 | 0.06 | 25,25,25,25                 | 0     |
| 54  | MG   | DB    | 3039 | 1/1   | 1.00 | 0.06 | 5,5,5,5                     | 0     |
| 54  | MG   | AA    | 1610 | 1/1   | 1.00 | 0.09 | 10,10,10,10                 | 0     |
| 54  | MG   | DB    | 3041 | 1/1   | 1.00 | 0.05 | 29,29,29,29                 | 0     |

*Continued on next page...*



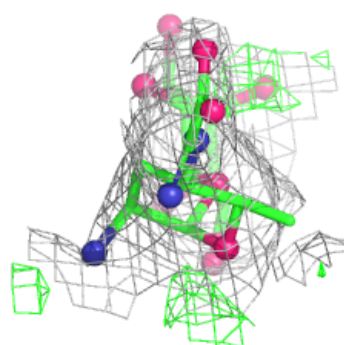
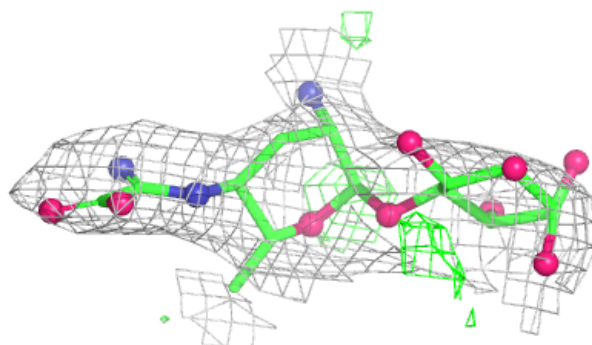
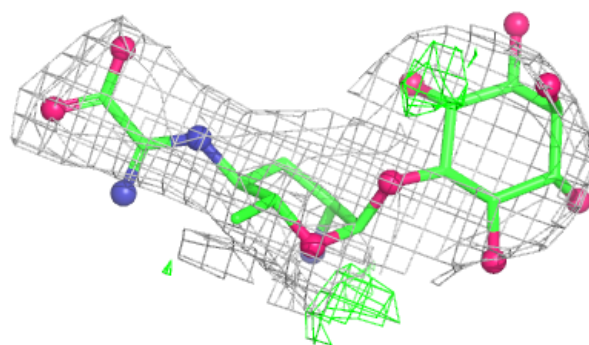
*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | CA    | 1611 | 1/1   | 1.00 | 0.02 | 43,43,43,43                 | 0     |
| 54  | MG   | DB    | 3043 | 1/1   | 1.00 | 0.03 | 7,7,7,7                     | 0     |
| 54  | MG   | DB    | 3072 | 1/1   | 1.00 | 0.06 | 5,5,5,5                     | 0     |
| 54  | MG   | DB    | 3019 | 1/1   | 1.00 | 0.03 | 8,8,8,8                     | 0     |
| 54  | MG   | DB    | 3074 | 1/1   | 1.00 | 0.05 | 12,12,12,12                 | 0     |
| 54  | MG   | BB    | 3037 | 1/1   | 1.00 | 0.07 | 21,21,21,21                 | 0     |
| 54  | MG   | CA    | 1602 | 1/1   | 1.00 | 0.06 | 8,8,8,8                     | 0     |
| 54  | MG   | DB    | 3022 | 1/1   | 1.00 | 0.03 | 5,5,5,5                     | 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.

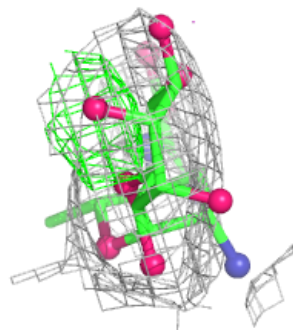
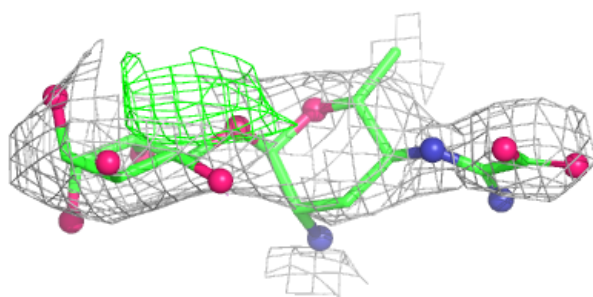
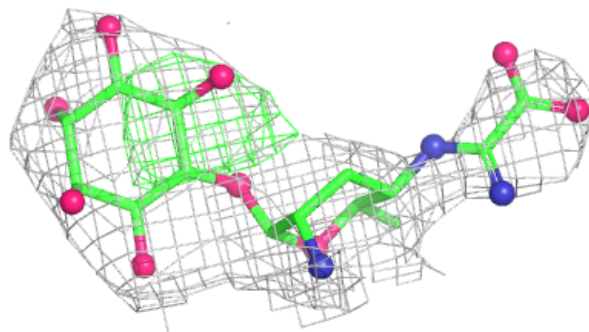
**Electron density around KSG AA 1601:**

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 KSG CA 1601:**

$2mF_o-DF_c$  (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.