



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2018 – 11:15 PM EST

PDB ID : 4V5F  
Title : The structure of the ribosome with elongation factor G trapped in the post-translocational state  
Authors : Gao, Y.-G.; Selmer, M.; Dunham, C.M.; Weixlbaumer, A.; Kelley, A.C.; Ramakrishnan, V.  
Deposited on : 2009-09-01  
Resolution : 3.60 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

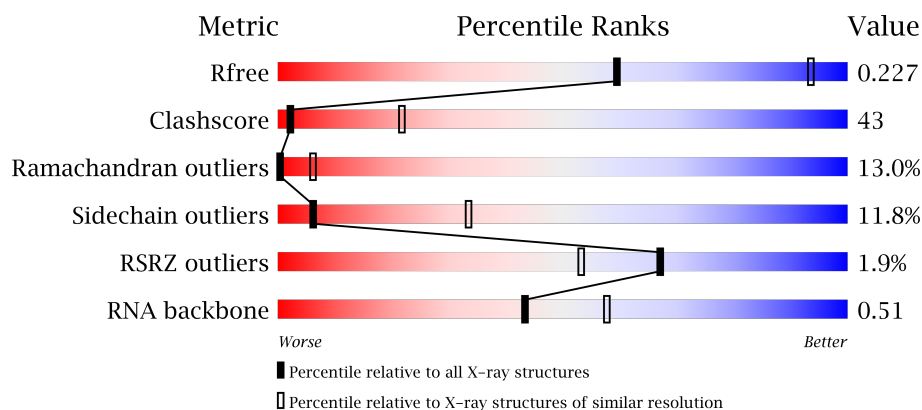
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



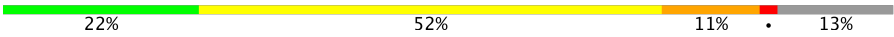
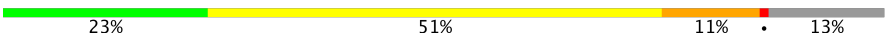



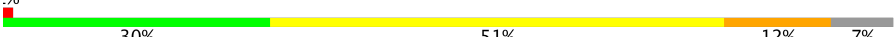
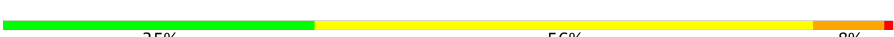
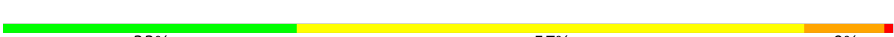
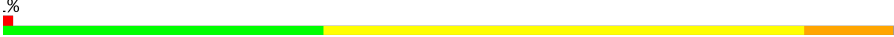

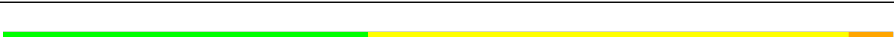
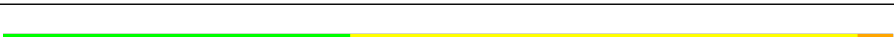

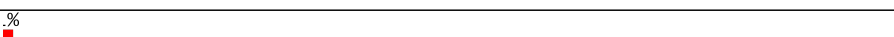
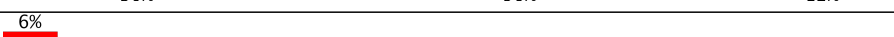
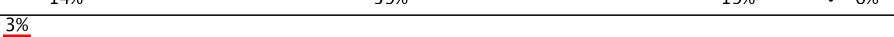



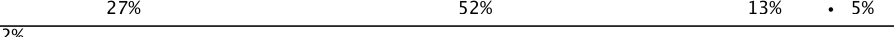
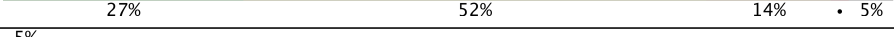
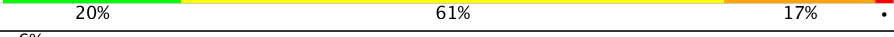
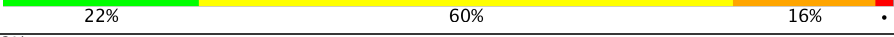


| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 100719                      | 1026 (3.74-3.46)                                      |
| Clashscore            | 112137                      | 1036 (3.70-3.50)                                      |
| Ramachandran outliers | 110173                      | 1030 (3.72-3.48)                                      |
| Sidechain outliers    | 110143                      | 1030 (3.72-3.48)                                      |
| RSRZ outliers         | 101464                      | 1051 (3.74-3.46)                                      |
| RNA backbone          | 2435                        | 1002 (4.30-2.90)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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    | 1522   | <div> <div>28%</div> <div>55%</div> <div>13%</div> <div>..</div> </div> |
| 1   | CA    | 1522   | <div> <div>27%</div> <div>57%</div> <div>14%</div> <div>..</div> </div> |
| 2   | AB    | 256    | <div> <div>24%</div> <div>50%</div> <div>16%</div> <div>8%</div> </div> |
| 2   | CB    | 256    | <div> <div>23%</div> <div>50%</div> <div>16%</div> <div>8%</div> </div> |


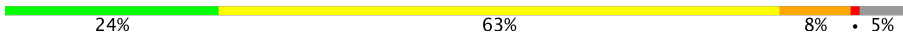
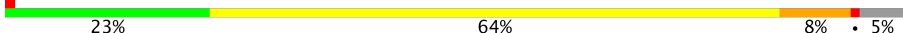


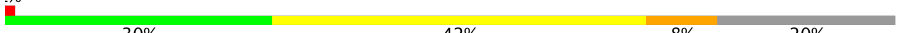
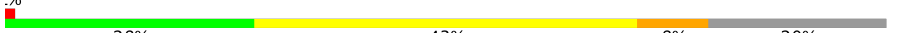




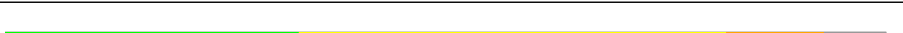





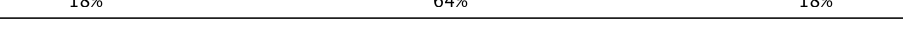


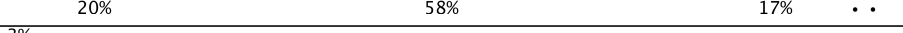
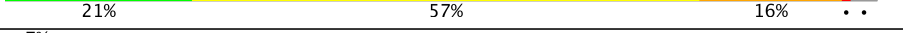


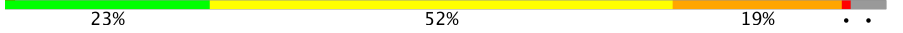
*Continued on next page...*

Continued from previous page...

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 3   | AC    | 239    |    |
| 3   | CC    | 239    |    |
| 4   | AD    | 209    |    |
| 4   | CD    | 209    |    |
| 5   | AE    | 162    |    |
| 5   | CE    | 162    |    |
| 6   | AF    | 101    |    |
| 6   | CF    | 101    |    |
| 7   | AG    | 156    |    |
| 7   | CG    | 156    |    |
| 8   | AH    | 138    |    |
| 8   | CH    | 138    |    |
| 9   | AI    | 128    |  |
| 9   | CI    | 128    |  |
| 10  | AJ    | 105    |  |
| 10  | CJ    | 105    |  |
| 11  | AK    | 129    |  |
| 11  | CK    | 129    |  |
| 12  | AL    | 132    |  |
| 12  | CL    | 132    |  |
| 13  | AM    | 126    |  |
| 13  | CM    | 126    |  |
| 14  | AN    | 61     |  |
| 14  | CN    | 61     |  |
| 15  | AO    | 89     |  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 15  | CO    | 89     |    |
| 16  | AP    | 88     |    |
| 16  | CP    | 88     |    |
| 17  | AQ    | 105    |    |
| 17  | CQ    | 105    |    |
| 18  | AR    | 88     |    |
| 18  | CR    | 88     |    |
| 19  | AS    | 93     |    |
| 19  | CS    | 93     |    |
| 20  | AT    | 106    |    |
| 20  | CT    | 106    |    |
| 21  | AU    | 27     |    |
| 21  | CU    | 27     |  |
| 22  | AV    | 77     |  |
| 22  | AW    | 77     |  |
| 22  | CV    | 77     |  |
| 22  | CW    | 77     |  |
| 23  | AX    | 25     |  |
| 23  | CX    | 25     |  |
| 24  | AY    | 691    |  |
| 24  | CY    | 691    |  |
| 25  | B0    | 85     |  |
| 25  | D0    | 85     |  |
| 26  | B1    | 98     |  |
| 26  | D1    | 98     |  |

Continued on next page...



Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 27  | B2    | 72     |                  |
| 27  | D2    | 72     |                  |
| 28  | B3    | 60     |                  |
| 28  | D3    | 60     |                  |
| 29  | B4    | 71     |                  |
| 29  | D4    | 71     |                  |
| 30  | B5    | 60     |                  |
| 30  | D5    | 60     |                  |
| 31  | B6    | 54     |                  |
| 31  | D6    | 54     |                  |
| 32  | B7    | 49     |                  |
| 32  | D7    | 49     |                  |
| 33  | B8    | 65     |                  |
| 33  | D8    | 65     |                  |
| 34  | B9    | 37     |                  |
| 34  | D9    | 37     |                  |
| 35  | BA    | 2915   |                  |
| 35  | DA    | 2915   |                  |
| 36  | BB    | 122    |                  |
| 36  | DB    | 122    |                  |
| 37  | BC    | 229    |                  |
| 37  | DC    | 229    |                  |
| 38  | BD    | 276    |                  |
| 38  | DD    | 276    |                  |
| 39  | BE    | 206    |                  |



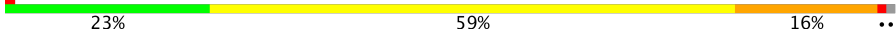
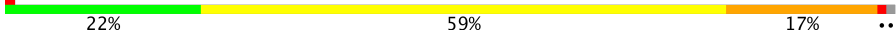
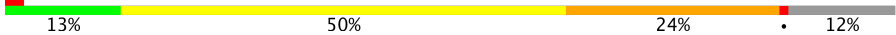
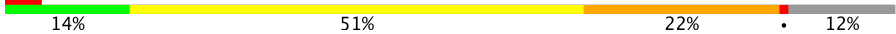
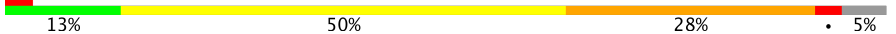
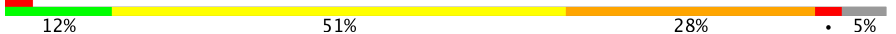
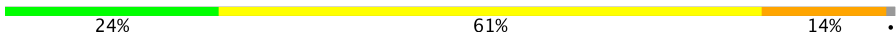
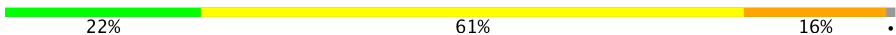
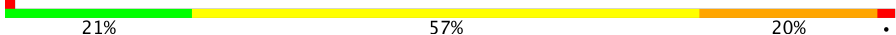

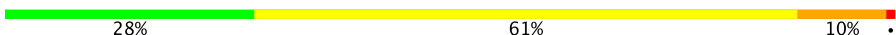







Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 39  | DE    | 206    |                  |
| 40  | BF    | 210    |                  |
| 40  | DF    | 210    |                  |
| 41  | BG    | 182    |                  |
| 41  | DG    | 182    |                  |
| 42  | BH    | 180    |                  |
| 42  | DH    | 180    |                  |
| 43  | BJ    | 173    |                  |
| 43  | DJ    | 173    |                  |
| 44  | BK    | 147    |                  |
| 44  | DK    | 147    |                  |
| 45  | BL    | 125    |                  |
| 45  | BM    | 125    |                  |
| 45  | Bl    | 125    |                  |
| 45  | Bm    | 125    |                  |
| 45  | DL    | 125    |                  |
| 45  | DM    | 125    |                  |
| 45  | Dl    | 125    |                  |
| 45  | Dm    | 125    |                  |
| 46  | BN    | 140    |                  |
| 46  | DN    | 140    |                  |
| 47  | BO    | 122    |                  |
| 47  | DO    | 122    |                  |
| 48  | BP    | 150    |                  |
| 48  | DP    | 150    |                  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 49  | BQ    | 141    |    |
| 49  | DQ    | 141    |    |
| 50  | BR    | 118    |    |
| 50  | DR    | 118    |    |
| 51  | BS    | 112    |    |
| 51  | DS    | 112    |    |
| 52  | BT    | 146    |    |
| 52  | DT    | 146    |    |
| 53  | BU    | 118    |    |
| 53  | DU    | 118    |    |
| 54  | BV    | 101    |    |
| 54  | DV    | 101    |   |
| 55  | BW    | 113    |  |
| 55  | DW    | 113    |  |
| 56  | BX    | 96     |  |
| 56  | DX    | 96     |  |
| 57  | BY    | 110    |  |
| 57  | DY    | 110    |  |
| 58  | BZ    | 206    |  |
| 58  | DZ    | 206    |  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 61  | FUA  | AY    | 702 | -         | -        | -       | X                |
| 61  | FUA  | CY    | 702 | -         | -        | X       | -                |

## 2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 311552 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    | 1504     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32329 | 14390 | 5992 | 10444 | 1503 |         |         |       |
| 1   | CA    | 1504     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32329 | 14390 | 5992 | 10444 | 1503 |         |         |       |

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | AB    | 235      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1901  | 1213 | 342 | 341 | 5 |         |         |       |
| 2   | CB    | 235      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1901  | 1213 | 342 | 341 | 5 |         |         |       |

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | AC    | 207      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1613  | 1016 | 315 | 281 | 1 |         |         |       |
| 3   | CC    | 207      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1613  | 1016 | 315 | 281 | 1 |         |         |       |

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | AD    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1703  | 1066 | 339 | 291 | 7 |         |         |       |
| 4   | CD    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1703  | 1066 | 339 | 291 | 7 |         |         |       |

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | AE    | 151      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1147  | 724 | 218 | 201 | 4 |         |         |       |
| 5   | CE    | 151      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1147  | 724 | 218 | 201 | 4 |         |         |       |

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | AF    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 843   | 531 | 155 | 154 | 3 |         |         |       |
| 6   | CF    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 843   | 531 | 155 | 154 | 3 |         |         |       |

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | AG    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1257  | 781 | 252 | 218 | 6 |         |         |       |
| 7   | CG    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1257  | 781 | 252 | 218 | 6 |         |         |       |

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | AH    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1116  | 705 | 215 | 193 | 3 |         |         |       |
| 8   | CH    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1116  | 705 | 215 | 193 | 3 |         |         |       |

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 9   | AI    | 127      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1010  | 639 | 197 | 174 |  |         |         |       |
| 9   | CI    | 127      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1010  | 639 | 197 | 174 |  |         |         |       |

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | AJ    | 99       | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 795   | 499 | 157 | 138 | 1 |         |         |       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | CJ    | 99       | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 795   | 499 | 157 | 138 | 1 |         |         |       |

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | AK    | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 885   | 549 | 168 | 165 | 3 |         |         |       |
| 11  | CK    | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 885   | 549 | 168 | 165 | 3 |         |         |       |

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | AL    | 125      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 971   | 611 | 196 | 163 | 1 |         |         |       |
| 12  | CL    | 125      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 971   | 611 | 196 | 163 | 1 |         |         |       |

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | AM    | 125      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 988   | 611 | 206 | 169 | 2 |         |         |       |
| 13  | CM    | 125      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 988   | 611 | 206 | 169 | 2 |         |         |       |

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 14  | AN    | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 492   | 312 | 104 | 72 | 4 |         |         |       |
| 14  | CN    | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 492   | 312 | 104 | 72 | 4 |         |         |       |

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | AO    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 734   | 459 | 147 | 126 | 2 |         |         |       |
| 15  | CO    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 734   | 459 | 147 | 126 | 2 |         |         |       |

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | AP    | 84       | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 701   | 443 | 140 | 117 | 1 |         |         |       |
| 16  | CP    | 84       | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 701   | 443 | 140 | 117 | 1 |         |         |       |

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | AQ    | 100      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 824   | 528 | 152 | 142 | 2 |         |         |       |
| 17  | CQ    | 100      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 824   | 528 | 152 | 142 | 2 |         |         |       |

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 18  | AR    | 70       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 574   | 367 | 112 | 95 |         |         |       |
| 18  | CR    | 70       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 574   | 367 | 112 | 95 |         |         |       |

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | AS    | 79       | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 630   | 403 | 115 | 110 | 2 |         |         |       |
| 19  | CS    | 79       | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 630   | 403 | 115 | 110 | 2 |         |         |       |

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | AT    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 470 | 162 | 129 | 2 |         |         |       |
| 20  | CT    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 470 | 162 | 129 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21  | AU    | 25       | Total | C   | N  | O  | 0       | 0       | 1     |
|     |       |          | 209   | 128 | 51 | 30 |         |         |       |
| 21  | CU    | 25       | Total | C   | N  | O  | 0       | 0       | 1     |
|     |       |          | 209   | 128 | 51 | 30 |         |         |       |

- Molecule 22 is a RNA chain called E-SITE TRNA FMET OR P-SITE TRNA FMET (UN-MODIFIED BASES EXCEPT FOR THYMINE 54).

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 22  | AV    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1640  | 732 | 297 | 535 | 76 |         |         |       |
| 22  | AW    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1640  | 732 | 297 | 535 | 76 |         |         |       |
| 22  | CV    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1640  | 732 | 297 | 535 | 76 |         |         |       |
| 22  | CW    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1640  | 732 | 297 | 535 | 76 |         |         |       |

- Molecule 23 is a RNA chain called MRNA.

| Mol | Chain | Residues | Atoms |     |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 23  | AX    | 11       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 230   | 105 | 41 | 74 | 10 |         |         |       |
| 23  | CX    | 11       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 230   | 105 | 41 | 74 | 10 |         |         |       |

- Molecule 24 is a protein called ELONGATION FACTOR G.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 24  | AY    | 667      | Total | C    | N   | O   | S  | 0       | 0       | 1     |
|     |       |          | 5215  | 3316 | 893 | 988 | 18 |         |         |       |
| 24  | CY    | 667      | Total | C    | N   | O   | S  | 0       | 0       | 1     |
|     |       |          | 5215  | 3316 | 893 | 988 | 18 |         |         |       |

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 25  | B0    | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 662   | 410 | 140 | 111 | 1 |         |         |       |
| 25  | D0    | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 662   | 410 | 140 | 111 | 1 |         |         |       |

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.



| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26  | B1    | 94       | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 732   | 460 | 146 | 125 | 1 |         |         |       |
| 26  | D1    | 94       | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 732   | 460 | 146 | 125 | 1 |         |         |       |

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 27  | B2    | 71       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 598   | 370 | 121 | 106 | 1 |         |         |       |
| 27  | D2    | 71       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 598   | 370 | 121 | 106 | 1 |         |         |       |

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 28  | B3    | 60       | Total | C   | N  | O  | S | 0       | 0       | 1     |
|     |       |          | 468   | 298 | 91 | 78 | 1 |         |         |       |
| 28  | D3    | 60       | Total | C   | N  | O  | S | 0       | 0       | 1     |
|     |       |          | 468   | 298 | 91 | 78 | 1 |         |         |       |

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L31.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 29  | B4    | 58       | Total | C   | N  | O  | S | 0       | 0       | 1     |
|     |       |          | 451   | 285 | 78 | 83 | 5 |         |         |       |
| 29  | D4    | 58       | Total | C   | N  | O  | S | 0       | 0       | 1     |
|     |       |          | 451   | 285 | 78 | 83 | 5 |         |         |       |

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 30  | B5    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 459   | 288 | 90 | 76 | 5 |         |         |       |
| 30  | D5    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 459   | 288 | 90 | 76 | 5 |         |         |       |

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L33.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 31  | B6    | 50       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 433   | 270 | 88 | 71 | 4 |         |         |       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 31  | D6    | 50       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 433   | 270 | 88 | 71 | 4 |         |         |       |

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L34.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 32  | B7    | 49       | Total | C   | N   | O  | S | 0       | 0       | 1     |
|     |       |          | 419   | 257 | 105 | 55 | 2 |         |         |       |
| 32  | D7    | 49       | Total | C   | N   | O  | S | 0       | 0       | 1     |
|     |       |          | 419   | 257 | 105 | 55 | 2 |         |         |       |

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 33  | B8    | 64       | Total | C   | N   | O  | S | 0       | 0       | 1     |
|     |       |          | 508   | 326 | 102 | 78 | 2 |         |         |       |
| 33  | D8    | 64       | Total | C   | N   | O  | S | 0       | 0       | 1     |
|     |       |          | 508   | 326 | 102 | 78 | 2 |         |         |       |

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 34  | B9    | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 307   | 188 | 68 | 47 | 4 |         |         |       |
| 34  | D9    | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 307   | 188 | 68 | 47 | 4 |         |         |       |

- Molecule 35 is a RNA chain called 23S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 35  | BA    | 2901     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 62474 | 27806 | 11681 | 20087 | 2900 |         |         |       |
| 35  | DA    | 2901     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 62474 | 27806 | 11681 | 20087 | 2900 |         |         |       |

- Molecule 36 is a RNA chain called 5S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 36  | BB    | 119      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2551  | 1136 | 471 | 826 | 118 |         |         |       |
| 36  | DB    | 119      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2551  | 1136 | 471 | 826 | 118 |         |         |       |

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L1.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 37  | BC    | 228      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1742  | 1101 | 319 | 319 | 3 |         |         |       |
| 37  | DC    | 228      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1742  | 1101 | 319 | 319 | 3 |         |         |       |

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 38  | BD    | 275      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2145  | 1353 | 428 | 361 | 3 |         |         |       |
| 38  | DD    | 275      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2145  | 1353 | 428 | 361 | 3 |         |         |       |

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39  | BE    | 205      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1564  | 988 | 300 | 270 | 6 |         |         |       |
| 39  | DE    | 205      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1564  | 988 | 300 | 270 | 6 |         |         |       |

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 40  | BF    | 208      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1624  | 1035 | 304 | 282 | 3 |         |         |       |
| 40  | DF    | 208      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1624  | 1035 | 304 | 282 | 3 |         |         |       |

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41  | BG    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1474  | 942 | 268 | 260 | 4 |         |         |       |
| 41  | DG    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1474  | 942 | 268 | 260 | 4 |         |         |       |

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | BH    | 167      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1269  | 803 | 238 | 227 | 1 |         |         |       |
| 42  | DH    | 167      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1269  | 803 | 238 | 227 | 1 |         |         |       |

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L10.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43  | BJ    | 170      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 851   | 510 | 170 | 171 |   |         |         |       |
| 43  | DJ    | 170      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 851   | 510 | 170 | 171 |   |         |         |       |

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44  | BK    | 140      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1026  | 653 | 182 | 186 | 5 |         |         |       |
| 44  | DK    | 140      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1026  | 653 | 182 | 186 | 5 |         |         |       |

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L12.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 45  | BL    | 102      | Total | C   | N   | O   |  | 0       | 0       | 1     |
|     |       |          | 506   | 303 | 102 | 101 |  |         |         |       |
| 45  | BM    | 31       | Total | C   | N   | O   |  | 0       | 0       | 1     |
|     |       |          | 151   | 90  | 31  | 30  |  |         |         |       |
| 45  | Bl    | 31       | Total | C   | N   | O   |  | 0       | 0       | 1     |
|     |       |          | 151   | 90  | 31  | 30  |  |         |         |       |
| 45  | Bm    | 30       | Total | C   | N   | O   |  | 0       | 0       | 1     |
|     |       |          | 146   | 87  | 30  | 29  |  |         |         |       |
| 45  | DL    | 102      | Total | C   | N   | O   |  | 0       | 0       | 1     |
|     |       |          | 506   | 303 | 102 | 101 |  |         |         |       |
| 45  | DM    | 31       | Total | C   | N   | O   |  | 0       | 0       | 1     |
|     |       |          | 151   | 90  | 31  | 30  |  |         |         |       |
| 45  | Dl    | 31       | Total | C   | N   | O   |  | 0       | 0       | 1     |
|     |       |          | 151   | 90  | 31  | 30  |  |         |         |       |
| 45  | Dm    | 30       | Total | C   | N   | O   |  | 0       | 0       | 1     |
|     |       |          | 146   | 87  | 30  | 29  |  |         |         |       |

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46  | BN    | 139      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1105  | 712 | 207 | 182 | 4 |         |         |       |
| 46  | DN    | 139      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1105  | 712 | 207 | 182 | 4 |         |         |       |

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47  | BO    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |
| 47  | DO    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48  | BP    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1114  | 692 | 227 | 193 | 2 |         |         |       |
| 48  | DP    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1114  | 692 | 227 | 193 | 2 |         |         |       |

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 49  | BQ    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 715 | 212 | 188 | 7 |         |         |       |
| 49  | DQ    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 715 | 212 | 188 | 7 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 50  | BR    | 117      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 960   | 599 | 202 | 159 |  |         |         |       |
| 50  | DR    | 117      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 960   | 599 | 202 | 159 |  |         |         |       |

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L18.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 51  | BS    | 99       | Total | C   | N   | O   |  | 0       | 0       | 1     |
|     |       |          | 771   | 486 | 155 | 130 |  |         |         |       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 51  | DS    | 99       | Total | C   | N   | O   | 0       | 0       | 1     |
|     |       |          | 771   | 486 | 155 | 130 |         |         |       |

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 52  | BT    | 138      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1142  | 710 | 235 | 196 | 1 |         |         |       |
| 52  | DT    | 138      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1142  | 710 | 235 | 196 | 1 |         |         |       |

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 53  | BU    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 958   | 604 | 202 | 151 | 1 |         |         |       |
| 53  | DU    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 958   | 604 | 202 | 151 | 1 |         |         |       |

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 54  | BV    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 779   | 501 | 142 | 135 | 1 |         |         |       |
| 54  | DV    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 779   | 501 | 142 | 135 | 1 |         |         |       |

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 55  | BW    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 896   | 563 | 176 | 155 | 2 |         |         |       |
| 55  | DW    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 896   | 563 | 176 | 155 | 2 |         |         |       |

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L23.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 56  | BX    | 93       | Total | C   | N   | O   | 0       | 0       | 1     |
|     |       |          | 726   | 471 | 132 | 123 |         |         |       |
| 56  | DX    | 93       | Total | C   | N   | O   | 0       | 0       | 1     |
|     |       |          | 726   | 471 | 132 | 123 |         |         |       |

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 57  | BY    | 107      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 811   | 520 | 155 | 131 | 5 |         |         |       |
| 57  | DY    | 107      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 811   | 520 | 155 | 131 | 5 |         |         |       |

- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 58  | BZ    | 185      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1468  | 936 | 262 | 268 | 2 |         |         |       |
| 58  | DZ    | 185      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1468  | 936 | 262 | 268 | 2 |         |         |       |

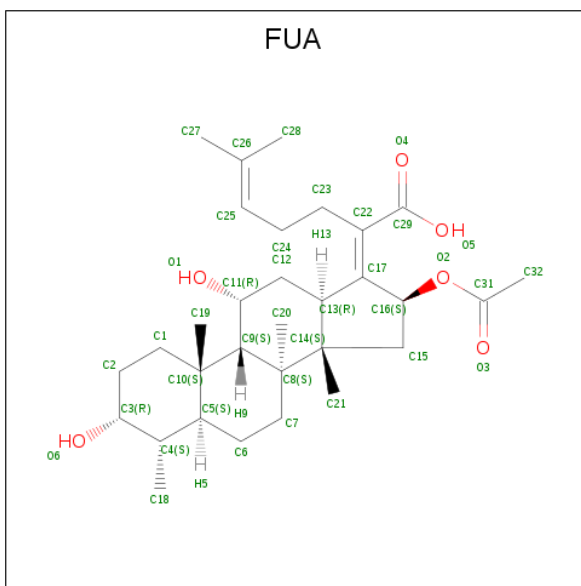
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 59  | B4    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | CN    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | AN    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | B9    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | D9    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | D4    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | CD    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | AD    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

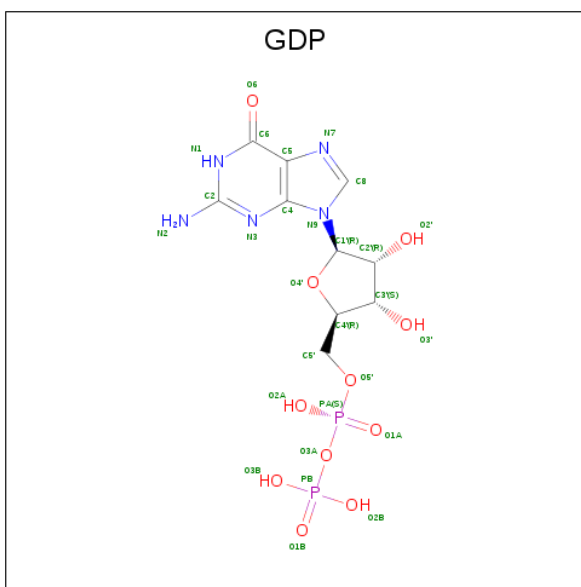
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 60  | AY    | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 60  | CY    | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 61 is FUSIDIC ACID (three-letter code: FUA) (formula:  $C_{31}H_{48}O_6$ ).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 61  | AY    | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 37    | 31 | 6 |         |         |
| 61  | CY    | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 37    | 31 | 6 |         |         |

- Molecule 62 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



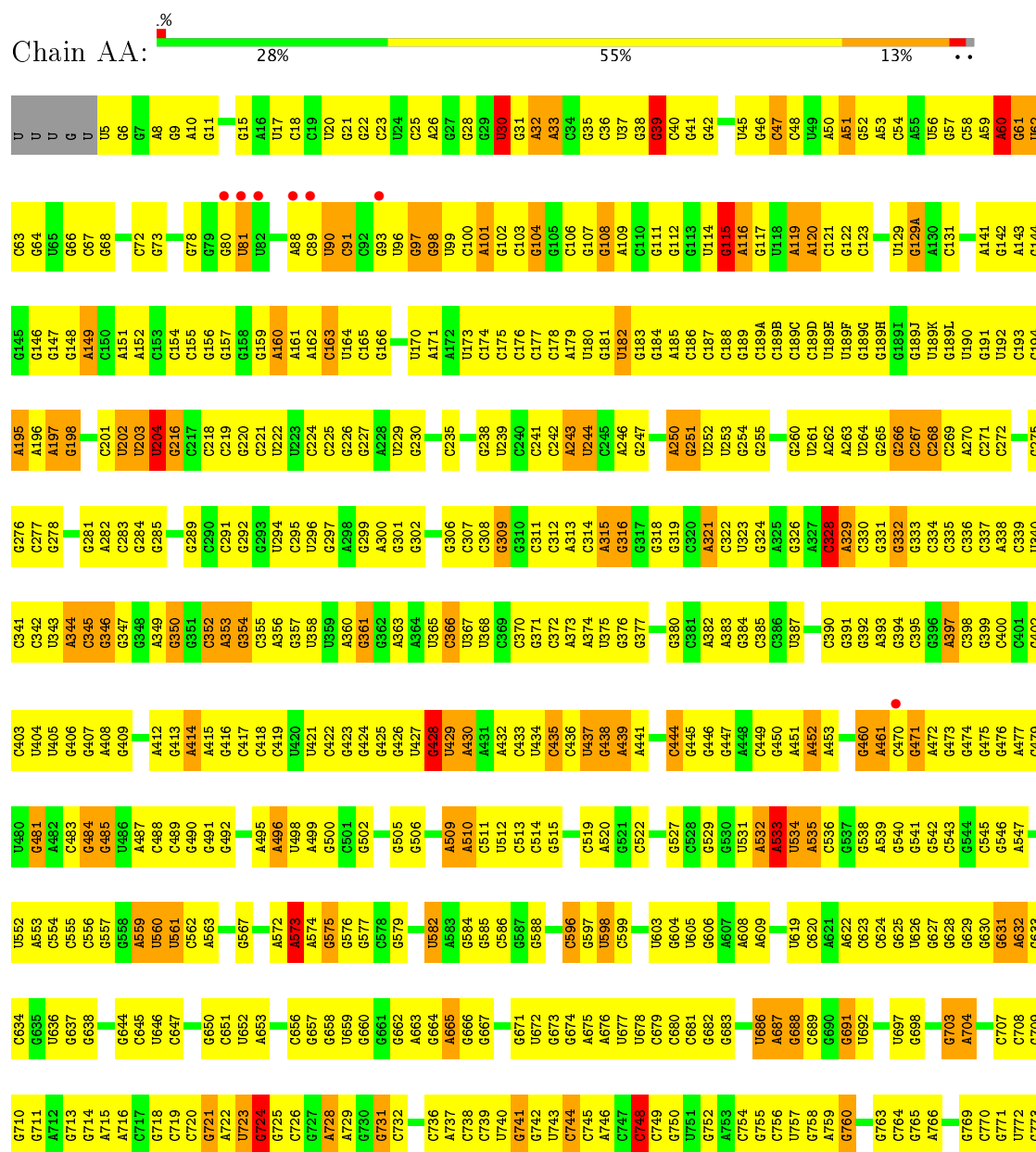


| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 62  | AY    | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |         |
| 62  | CY    | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |         |

### 3 Residue-property plots

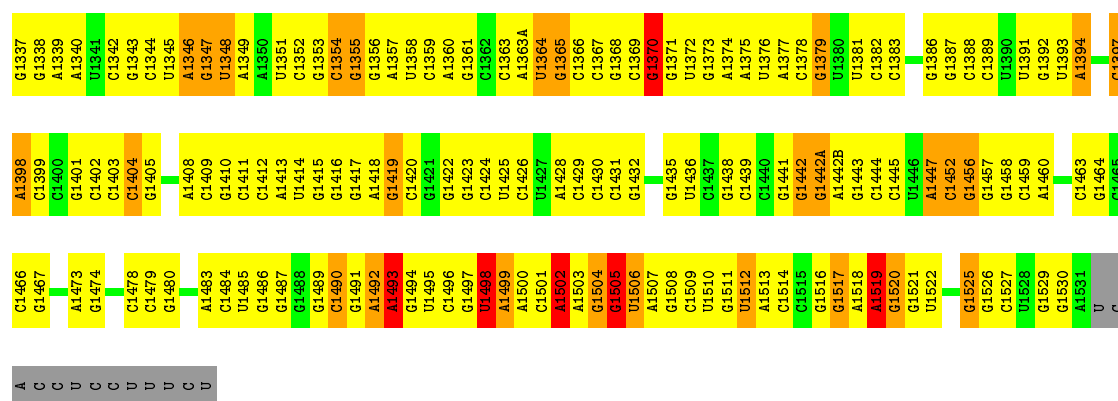
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ( $\text{RSRZ} > 2$ ). 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

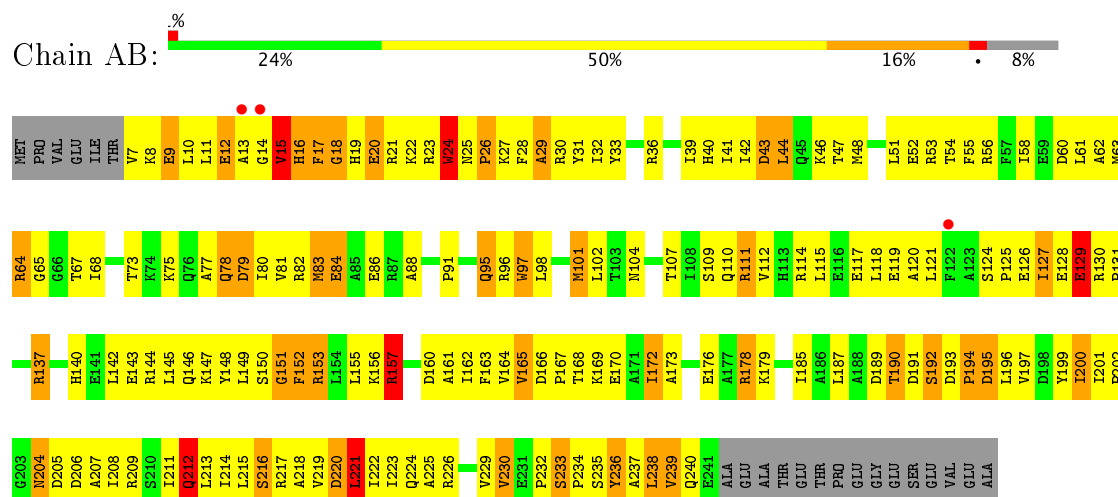




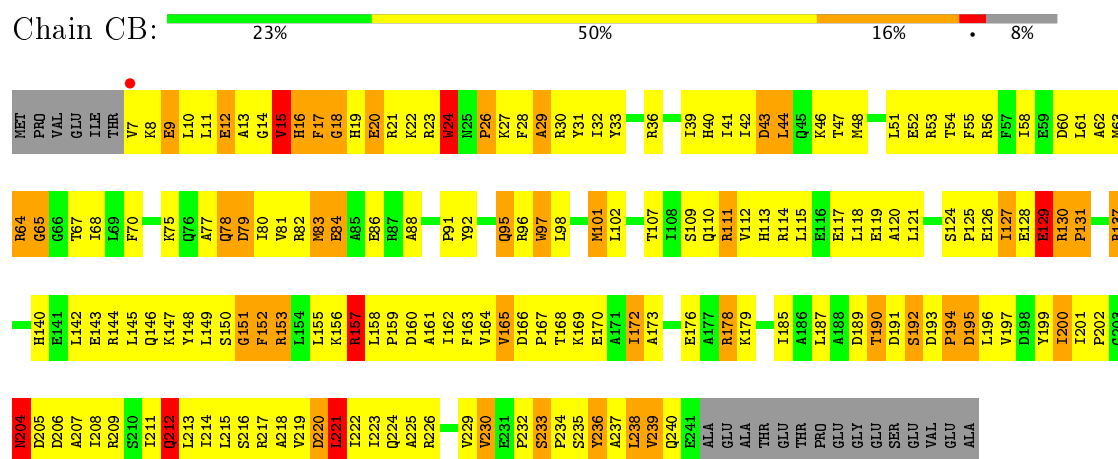
|       |       |       |        |       |      |      |      |      |      |      |      |      |      |      |
|-------|-------|-------|--------|-------|------|------|------|------|------|------|------|------|------|------|
| G1277 | U1211 | G1143 | G1001A | G939  | G854 | G778 | A712 | G638 | C556 | U486 | A408 | A344 | G278 | A195 |
| U1278 | U1212 | G1144 | G1002  | C940  | G858 | G779 | G713 | G641 | G557 | A487 | G409 | G345 | G281 | A196 |
| A1279 | A1213 | C1145 | G1003  | G941  | G859 | A780 | G714 | U641 | G558 | C488 | A412 | G346 | A282 | A197 |
| A1280 | C1214 | A1146 | A1004  | G942  | A859 | A781 | A715 | U646 | A559 | C489 | G413 | G347 | C283 | G198 |
| U1281 | G1215 | C1147 | A1005  | G943  | A860 | A782 | A716 | C647 | U560 | G490 | A414 | A348 | G284 | C201 |
| C1282 | G1216 | U1148 | C1006  | G944  | G861 | G783 | G717 | G650 | C562 | G492 | A415 | A349 | G285 | C201 |
| G1283 | C1217 | C1149 | C1007  | G945  | C862 | G784 | G718 | G650 | A572 | G495 | G416 | G351 | U202 | U202 |
| C1284 | U1150 | U1150 | G1008  | G946  | A865 | G785 | G719 | C651 | A573 | A496 | C417 | A352 | G289 | U204 |
| A1285 | G1009 | G1078 | G1009  | G947  | C866 | A787 | G720 | G652 | A574 | U498 | C418 | A353 | C290 | G216 |
| A1286 | A1151 | A1080 | A1010  | C948  | C867 | A788 | A722 | A653 | A575 | U499 | C419 | G354 | C291 | C217 |
| A1287 | C1153 | G1081 | G1082  | A949  | C868 | G791 | U723 | C656 | G575 | A500 | U420 | C355 | G292 | C218 |
| A1288 | G1154 | G1082 | A1014  | U950  | C874 | A792 | U724 | G657 | G576 | G501 | G421 | A356 | G293 | C219 |
| G1290 | U1083 | U1083 | A1015  | G951  | G874 | U793 | G725 | G658 | G577 | G502 | G422 | U358 | G294 | G220 |
| C1291 | A1157 | G1089 | A1016  | G953  | G878 | A794 | G726 | G659 | C578 | G505 | G423 | U359 | C295 | G221 |
| C1292 | C1158 | U1090 | C1018  | G954  | G879 | C796 | G727 | U659 | G579 | U359 | G424 | U360 | U296 | U222 |
| G1293 | U1159 | G1081 | C1019  | U955  | C879 | C796 | A728 | G660 | G582 | G505 | G425 | A360 | C297 | U223 |
| C1294 | C1160 | U1094 | U1020  | U956  | C880 | C797 | A729 | G661 | U582 | G506 | G428 | A361 | A298 | U223 |
| U1295 | C1161 | U1095 | U1021  | U957  | C882 | G797 | G730 | G662 | A583 | G509 | U429 | G362 | G299 | U229 |
| C1296 | C1162 | C1182 | U1025  | A958  | C883 | A802 | G731 | A663 | G584 | A509 | G428 | A363 | A300 | G230 |
| C1297 | G1123 | C1183 | G1026  | A959  | U884 | G803 | A732 | G664 | G585 | A510 | A431 | A364 | G301 | C235 |
| U1232 | U1232 | G1164 | A1101  | U960  | G885 |      | A733 | A665 | G586 | C511 | A432 | U365 | G302 |      |
| G1298 | C1233 | C1165 | C1028  | U961  | G886 | A807 | C736 | G666 | G588 | U512 | C433 | C366 |      |      |
| A1299 | A1300 | C1166 | C1029  | G962  | C887 | C808 |      | G667 |      | C513 | C434 | U367 | G306 | G238 |
| C1300 | C1234 | C1188 | G1030  | G963  |      |      | A737 |      | C596 | C514 | U434 | U368 | C307 | U239 |
| U1301 | U1235 | A1168 | A1105  | A964  | A892 | C811 | C738 | U672 | G597 | G515 | C435 | C369 | C308 | G240 |
| C1302 | C1236 | A1169 | G1030A | A965  | C893 | C812 | C739 | G673 | U598 | G520 | C436 | G370 | G309 | C241 |
| C1303 | C1237 | A1170 | C1030B | A966  | G894 | U813 | G740 | G674 | C599 | C519 | U437 | G371 | C310 | C242 |
| A1238 | G1171 | G1108 | G1030C | G967  | G895 | A814 | U741 | A675 | C602 | A521 | C438 | C372 | C311 | A243 |
| A1239 | C1172 | C1172 | A1030D | C967  | G896 | A815 | G742 | A676 | U602 | G521 | C439 | A373 | C312 | U244 |
| U1240 | G1173 | A1306 | G1031  | A968  | C896 | A815 | G742 | A676 | U603 | C522 | U439 | A373 | C312 | U244 |
| G1241 | G1174 | C1113 | G1032  | A969  | C897 | A816 | U743 | U677 | G604 | A522 | A441 | A374 | C313 | C245 |
| U1307 | C1175 | C1114 | G1033  | C970  | G898 | C817 | C744 | U678 | U605 | A523 | C444 | U375 | C314 | A246 |
| C1244 | A1176 | C1115 | G1034  | G971  | C899 | G818 |      | U679 | U606 | U534 | A451 | G376 | A315 | G247 |
| A1245 | A1179 | C1116 | A1035  | C972  | A900 | U820 | C747 | C680 | G606 | G527 | C445 | G377 | G316 |      |
| G1310 | G1117 | C1117 | G1036  | G973  | A901 | U820 | C748 | C681 | A607 | C528 | G446 |      | G317 | A250 |
| G1311 | C1118 | C1118 | C1037  | A974  | A902 | G821 | C749 | G682 | A608 | G529 | G447 | G380 | G318 | G251 |
| C1312 | C1119 | C1119 | C1038  | A975  | A903 | G822 | G750 | G683 | A609 | G530 | C448 | C381 | G319 | U252 |
| U1313 | G1184 | G1120 | C1039  | G976  | A904 | G823 | C751 | U686 | U610 | G531 | C449 | A382 | C320 | U253 |
| C1314 | A1251 | U1121 | G1047  | A977  | C910 | C824 | G752 | A687 | G617 | A532 | C450 | G383 | A321 | G254 |
| G1315 |       | U1121 | C1048  | A978  | C910 | C825 | C753 | G688 | G617 | U533 | C451 | G384 | C322 | G256 |
| C1316 | A1252 | U1122 | G1049  | C979  | A913 | C826 | G754 | U686 | G617 | A534 | A452 | C385 | U323 | U256 |
| G1317 | G1253 | C1123 | U1049  | C980  | A914 | U827 | C755 | G689 | U619 | A535 | A453 |      | G324 | G257 |
| C1254 | C1254 | G1124 | U1049  | C980  | A914 | U827 | C755 | G689 | U619 | A535 | A453 |      | G324 | G257 |
| A1255 | U1255 | U1125 | G1050  | U981  | A915 | A828 | C756 | G690 | C620 | C536 |      | C390 | A325 |      |
| C1320 | A1256 | U1126 | G1051  | U982  | U921 | G829 | G758 | G691 | A621 | G537 | G460 | G391 | G326 | G260 |
| U1257 | C1195 | G1127 | G1052  | A982  | G922 | G829 | G759 | G691 | A622 | G538 | A461 | G392 | A327 | U261 |
| C1322 | C1258 | C1128 | C1054  | A983  | A923 | U830 | G760 | U692 | A623 | G539 | C470 | A393 | C328 | A262 |
| G1323 | C1259 | G1197 | A1055  | A886  | C924 | C832 | G763 | G693 | C623 | A539 | C471 | A394 | A329 | A263 |
| C1260 | A1198 | A1130 | U1056  | G987  | G925 | U833 | C764 | A694 | C624 | G540 | G471 | G394 | C330 | U264 |
| A1325 | U1199 | G1131 | G1057  | G987  | G926 | U834 | G765 | A695 | G625 | G541 | A472 | C395 | G331 | G265 |
| C1326 | C1262 | C1132 | C1058  | U991  | G927 | C835 | G766 | U697 | U626 | C544 | G473 | A397 | G332 | G266 |
|       |       | G1133 | G1059  | U991  | G927 | U836 | A767 | G698 | G628 | G544 | G474 | C398 | G333 | C267 |
| A1266 | G1202 | G1134 | C1060  | G993  | C930 | G836 | G768 |      | G629 | C545 | G476 | G399 | C334 | C268 |
| A1269 | C1203 | U1135 | G1061  | A994  | C931 | U839 | A769 |      | G630 | G546 | A477 | C400 | C335 | C269 |
| C1270 | A1204 | U1062 | U1062  | C995  | C932 | C840 | C770 | A704 | G631 | A547 | C478 | C401 | C336 | A270 |
| G1271 | G1205 | C1137 | C1063  | A996  | G933 | U841 | G771 |      | A632 | G548 | U480 | G402 | C337 | C271 |
| G1272 | C1206 | G1138 | G1064  | U997  | C934 | C848 | U772 | C707 | G633 | U552 | G481 | C403 | A338 | C272 |
| G1273 | G1207 | G1139 | U1065  | G998  | A935 | G849 | G773 | G708 | C634 | A553 | A482 | U404 |      | G275 |
| C1274 | G1208 | C1140 | C1066  | C999  | C936 | G851 | G774 | G709 | G635 | C554 | A483 | U405 | C342 | G276 |
| A1275 | C1209 | U1141 | A1067  | U1000 | A937 | G852 | G775 | G710 | U636 | G555 | G484 | G406 | U343 | G277 |
| C1276 | C1142 | C1142 | G1068  | A1001 | A938 | G853 | A777 |      | G637 |      |      |      |      |      |



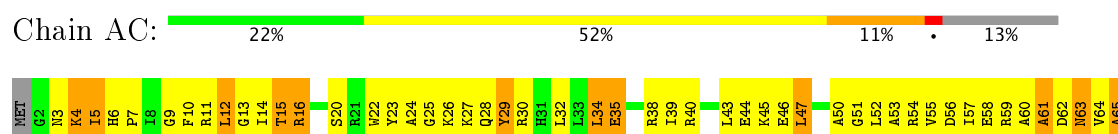
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

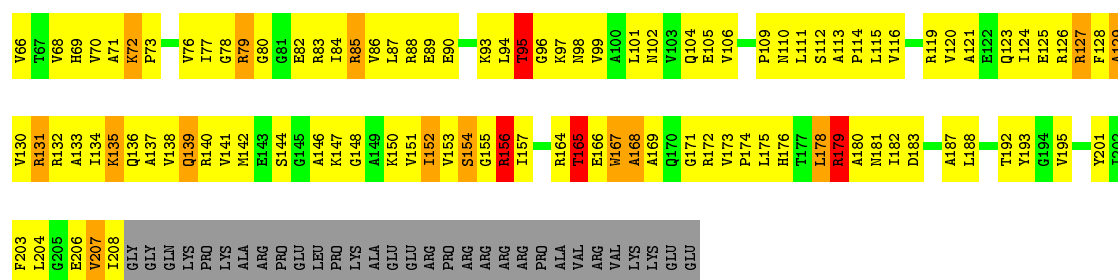


- Molecule 2: 30S RIBOSOMAL PROTEIN S2

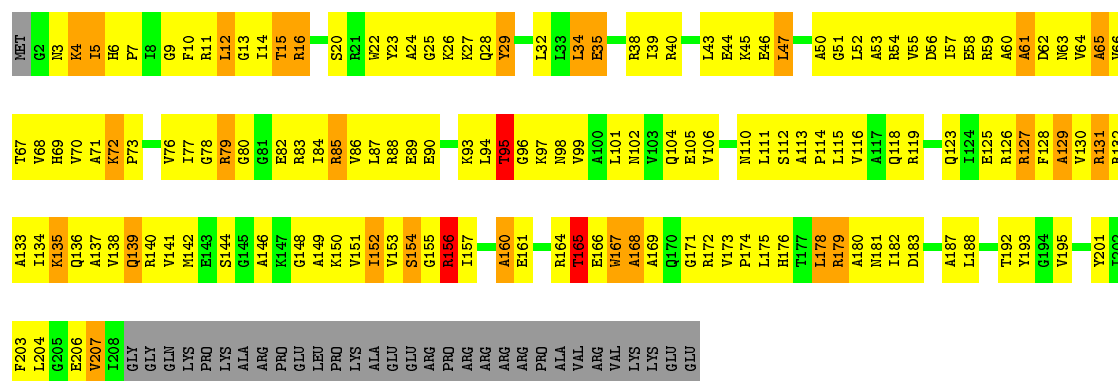


- Molecule 3: 30S RIBOSOMAL PROTEIN S3

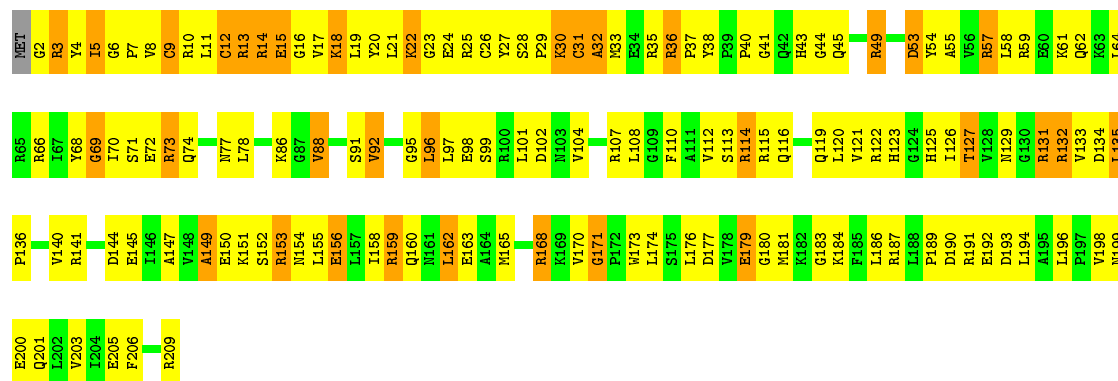




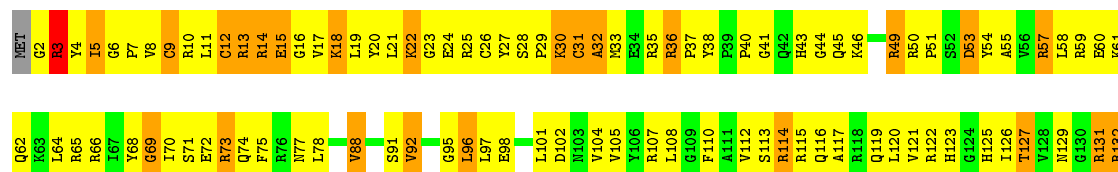
- Molecule 3: 30S RIBOSOMAL PROTEIN S3

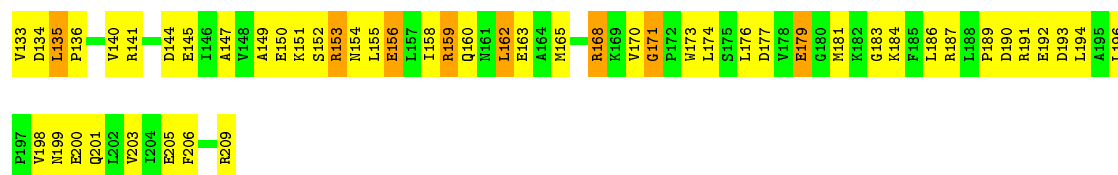


- Molecule 4: 30S RIBOSOMAL PROTEIN S4

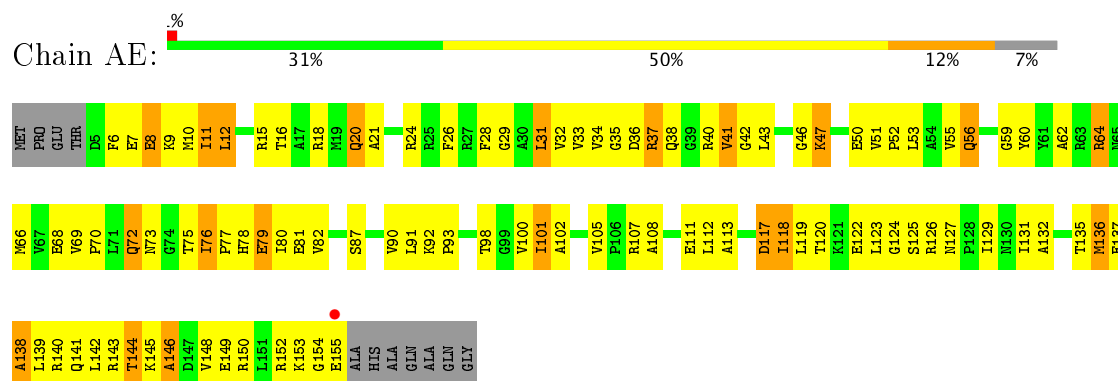


- Molecule 4: 30S RIBOSOMAL PROTEIN S4

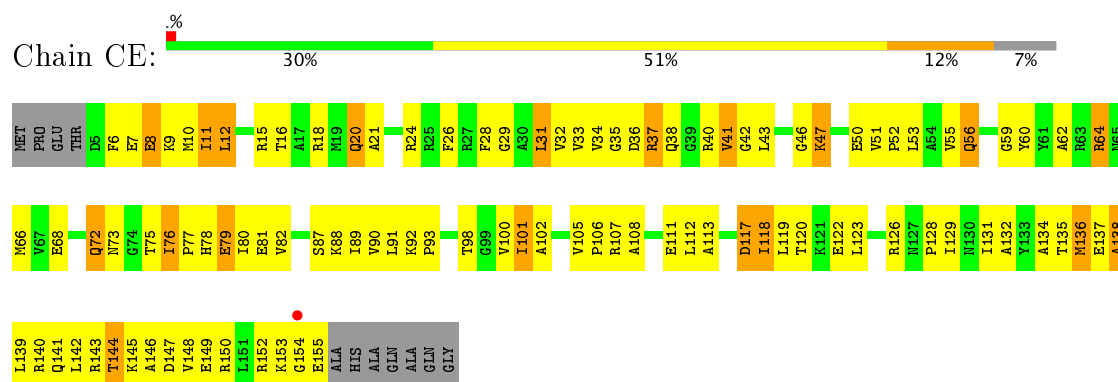




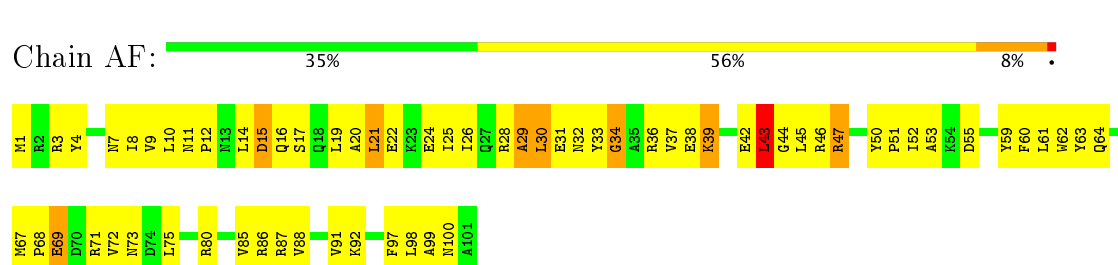
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



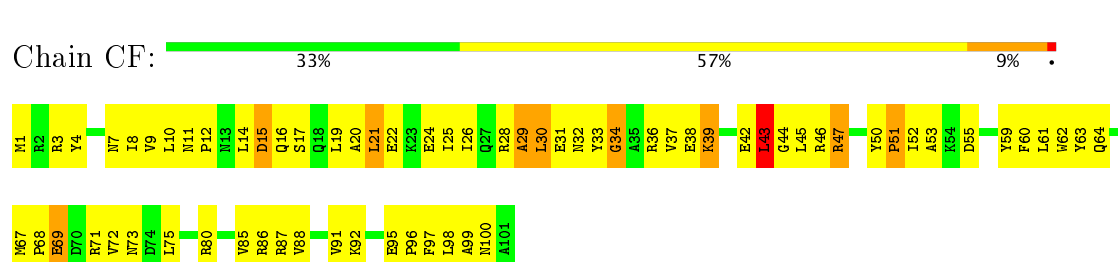
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



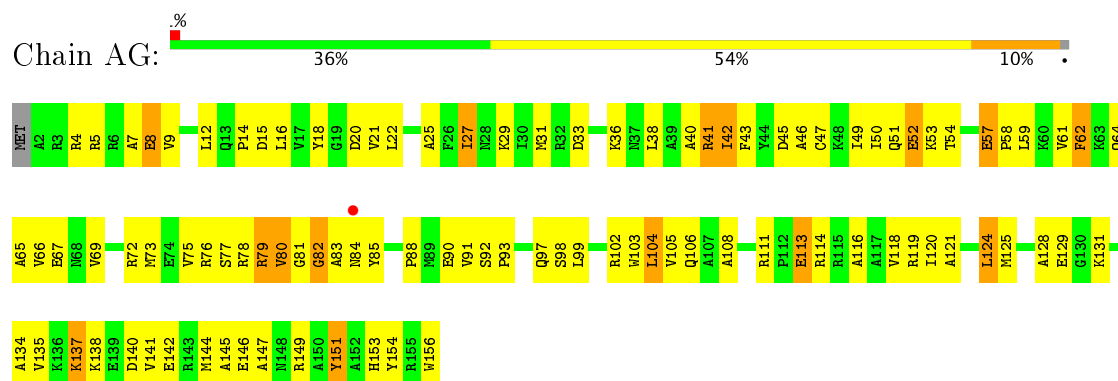
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



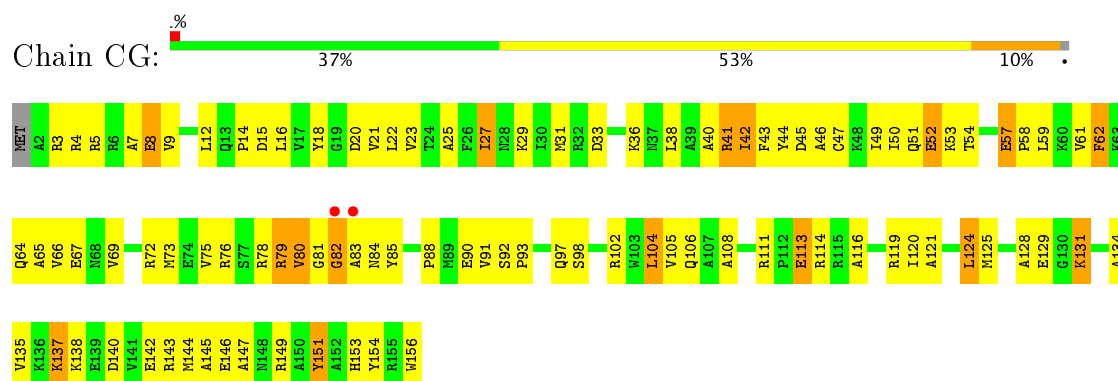
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



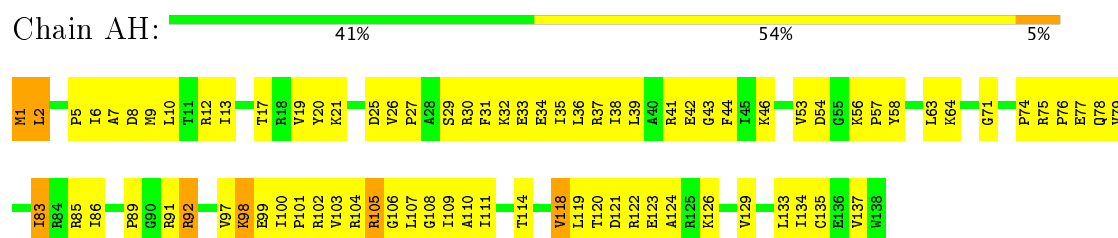
- Molecule 7: 30S RIBOSOMAL PROTEIN S7



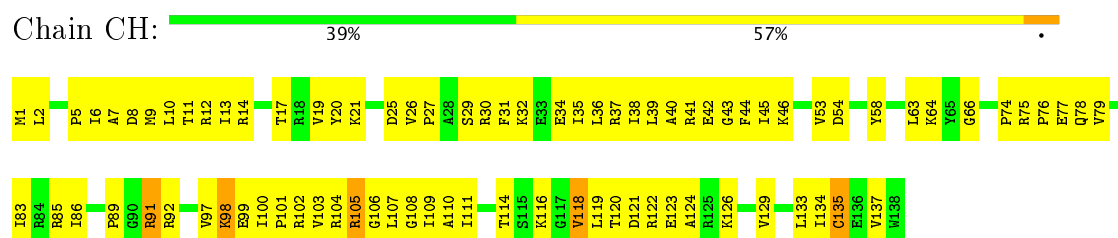
- Molecule 7: 30S RIBOSOMAL PROTEIN S7



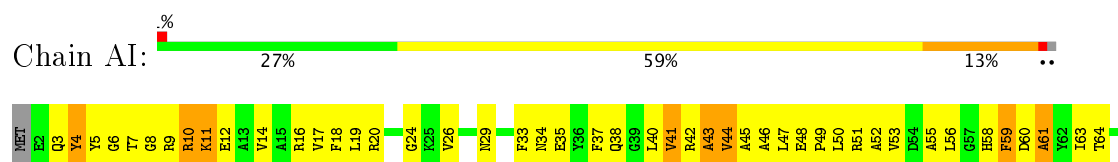
- Molecule 8: 30S RIBOSOMAL PROTEIN S8



- Molecule 8: 30S RIBOSOMAL PROTEIN S8



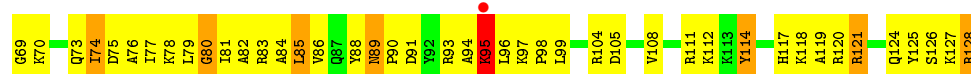
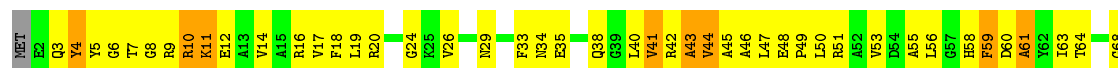
- Molecule 9: 30S RIBOSOMAL PROTEIN S9



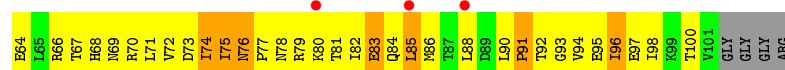
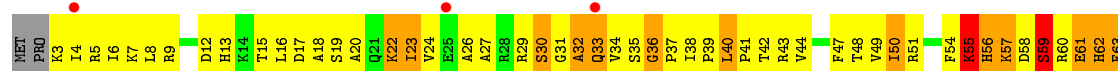
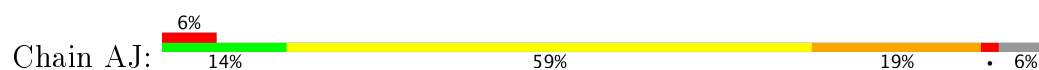




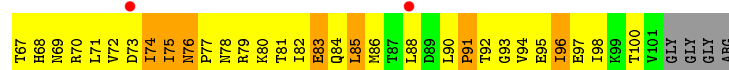
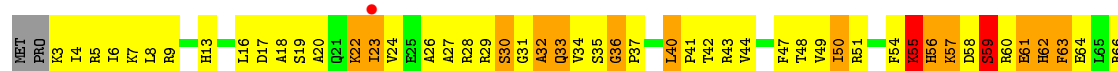
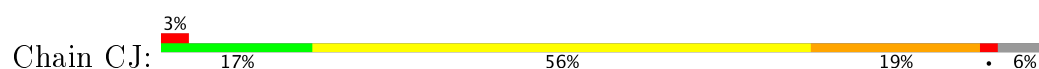
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



• Molecule 10: 30S RIBOSOMAL PROTEIN S10



• Molecule 10: 30S RIBOSOMAL PROTEIN S10



• Molecule 11: 30S RIBOSOMAL PROTEIN S11

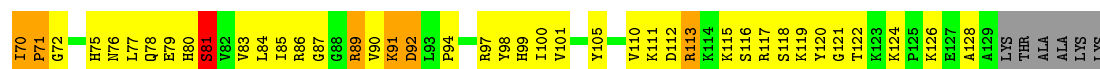
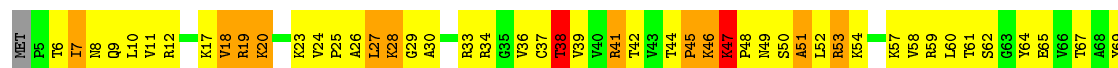


• Molecule 11: 30S RIBOSOMAL PROTEIN S11

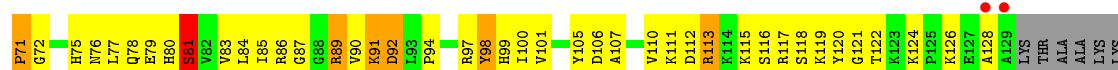
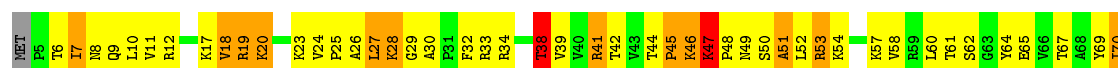




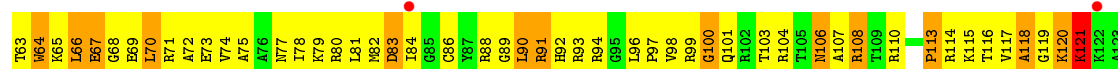
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



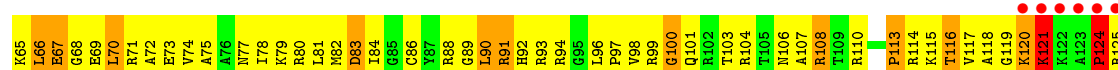
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



• Molecule 13: 30S RIBOSOMAL PROTEIN S13



• Molecule 13: 30S RIBOSOMAL PROTEIN S13



- Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain AN: 



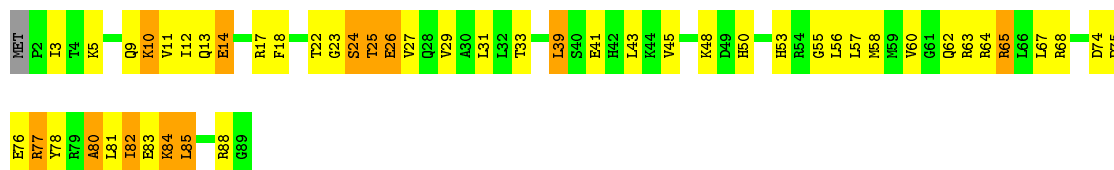
- Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain CN: 



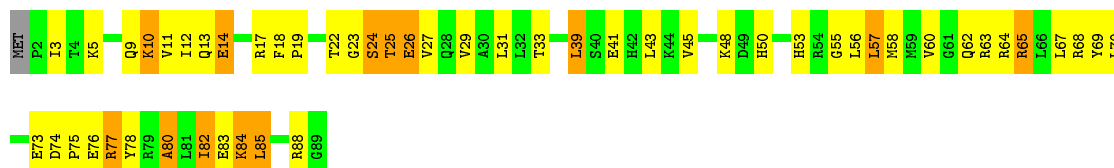
- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO: 



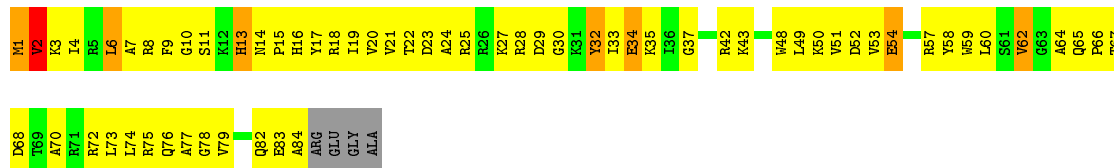
- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CO: 



- Molecule 16: 30S RIBOSOMAL PROTEIN S16

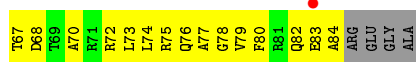
Chain AP: 



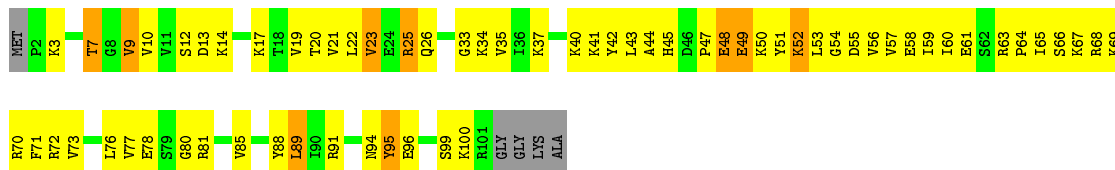
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CP: 

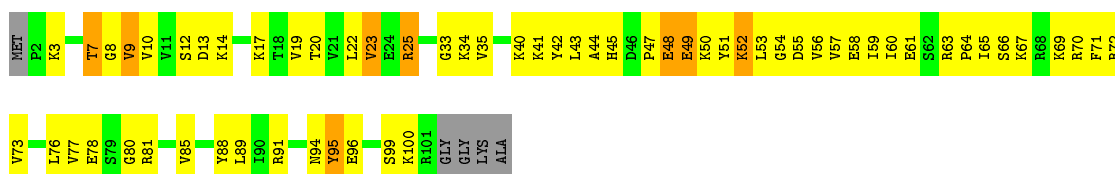




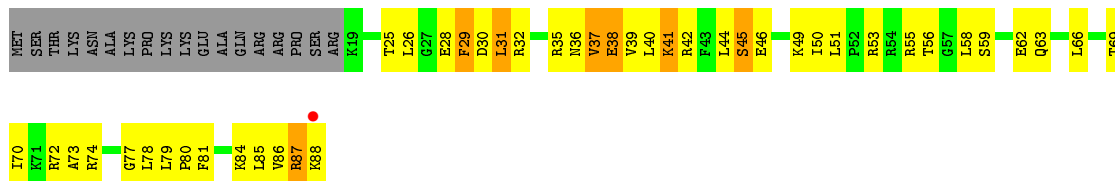
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



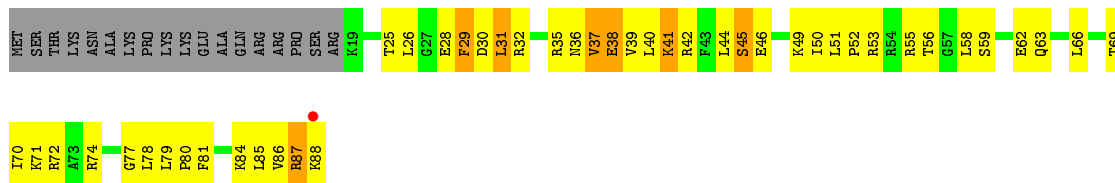
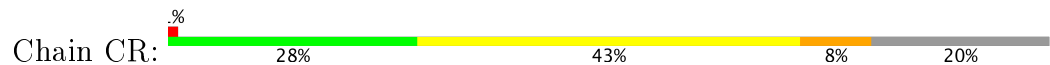
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



• Molecule 18: 30S RIBOSOMAL PROTEIN S18

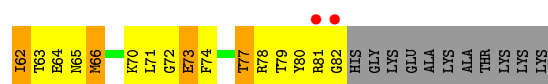


• Molecule 18: 30S RIBOSOMAL PROTEIN S18

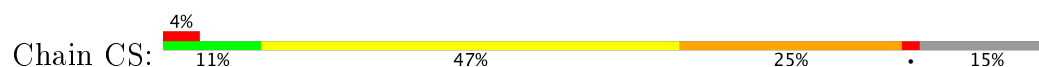


• Molecule 19: 30S RIBOSOMAL PROTEIN S19

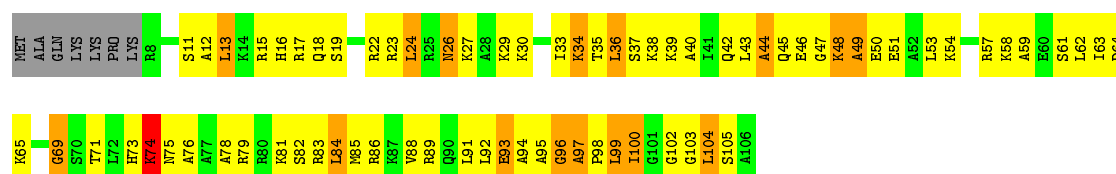


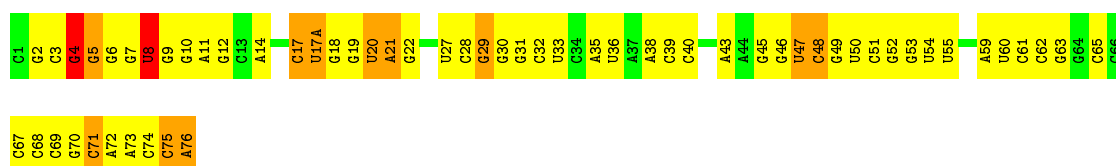


• Molecule 19: 30S RIBOSOMAL PROTEIN S19

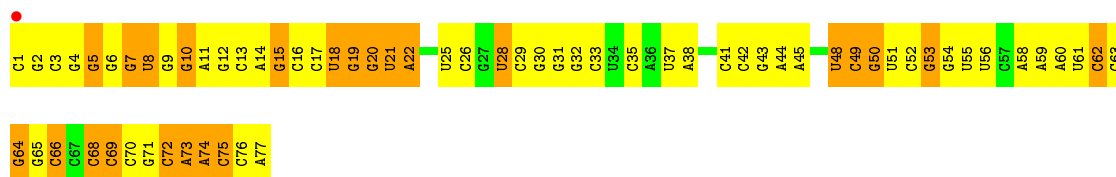
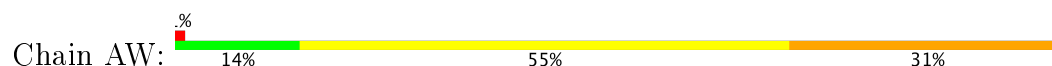


• Molecule 20: 30S RIBOSOMAL PROTEIN S20

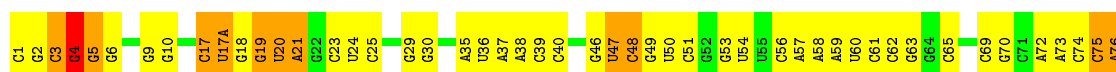




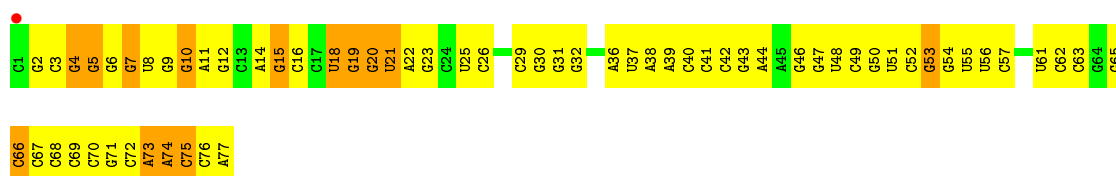
- Molecule 22: E-SITE TRNA FMET OR P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54)



- Molecule 22: E-SITE TRNA FMET OR P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54)



- Molecule 22: E-SITE TRNA FMET OR P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54)



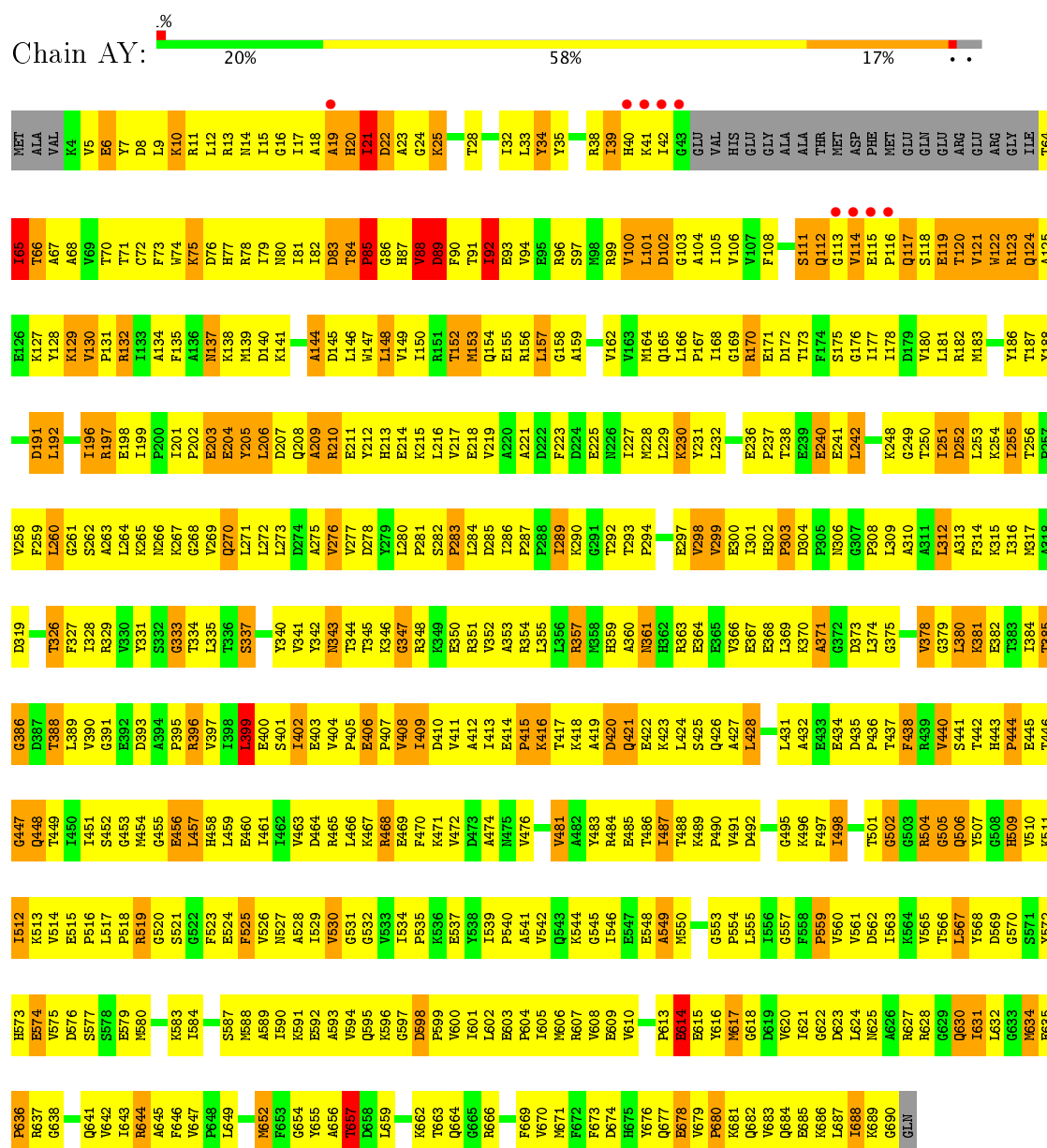
- Molecule 23: MRNA

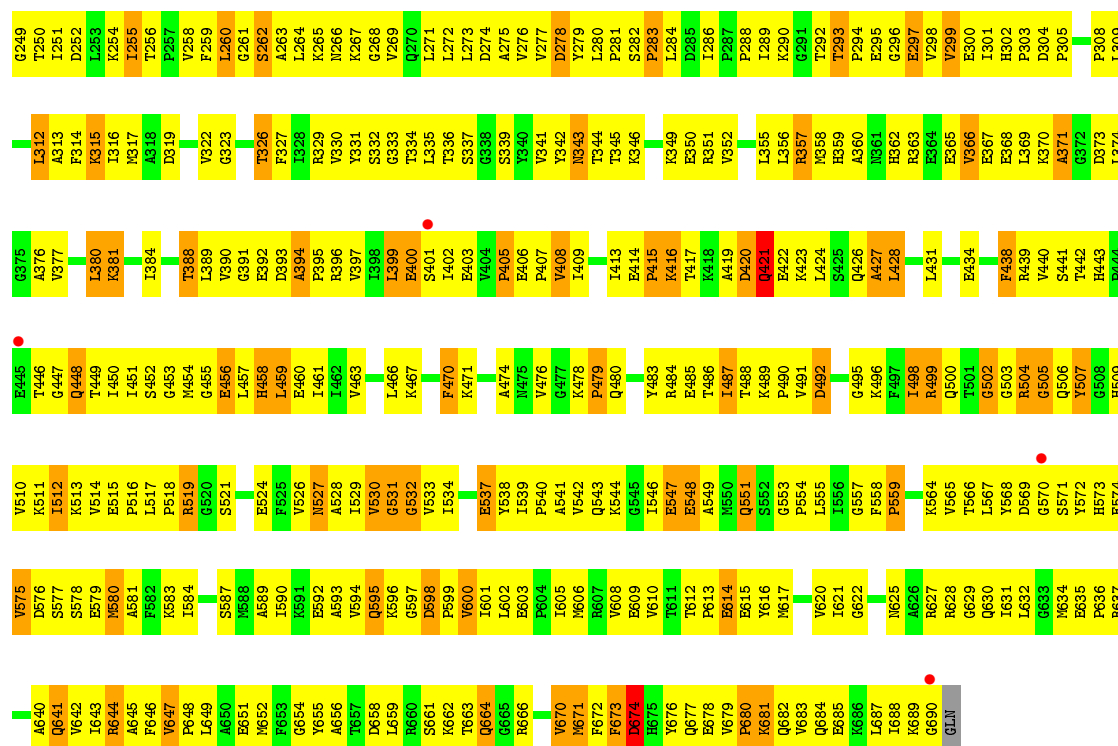


- Molecule 23: MRNA

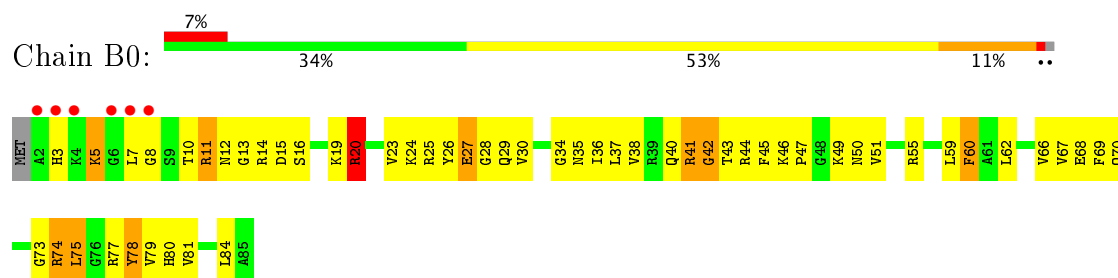


- Molecule 24: ELONGATION FACTOR G

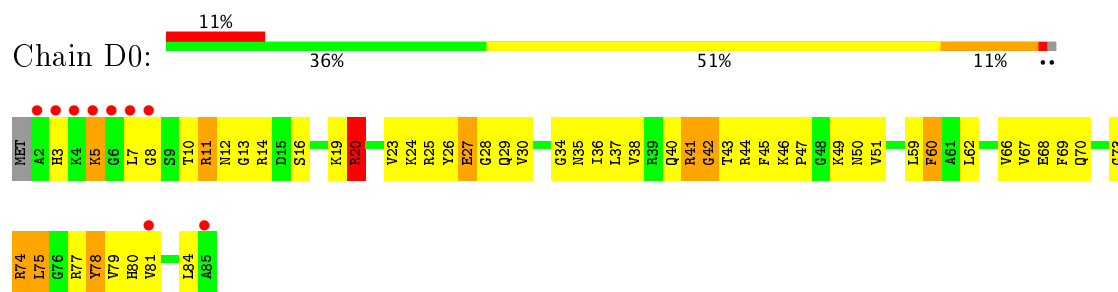




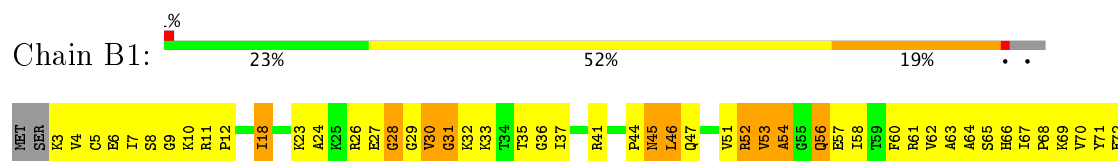
• Molecule 25: 50S RIBOSOMAL PROTEIN L27



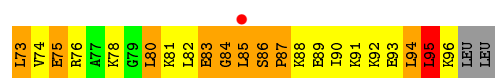
• Molecule 25: 50S RIBOSOMAL PROTEIN L27



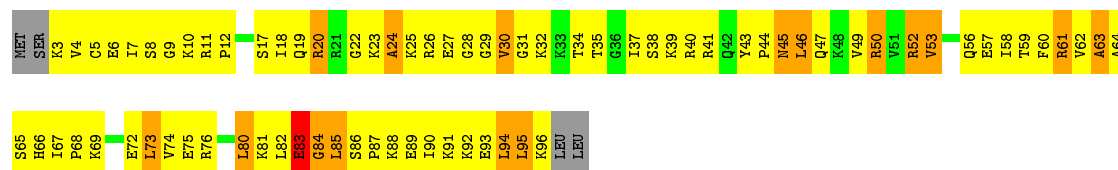
• Molecule 26: 50S RIBOSOMAL PROTEIN L28



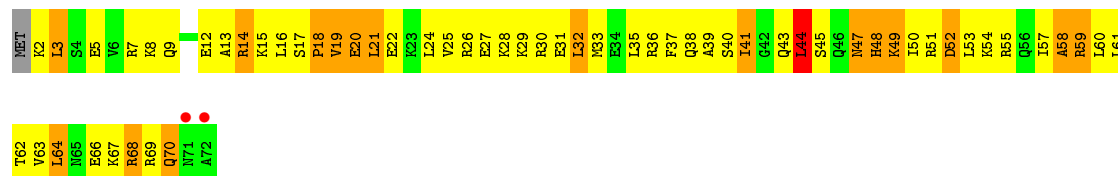




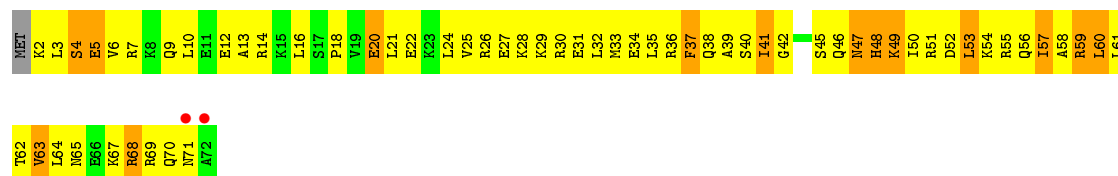
• Molecule 26: 50S RIBOSOMAL PROTEIN L28



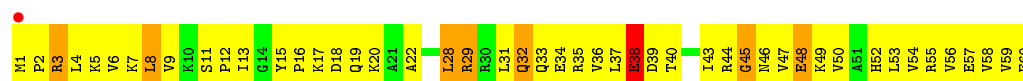
• Molecule 27: 50S RIBOSOMAL PROTEIN L29



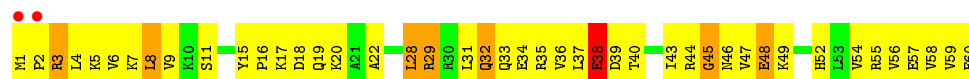
• Molecule 27: 50S RIBOSOMAL PROTEIN L29



• Molecule 28: 50S RIBOSOMAL PROTEIN L30

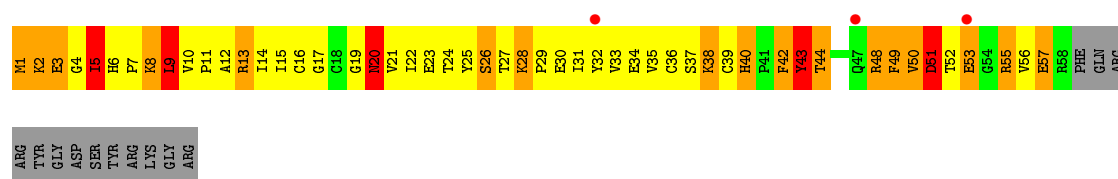


• Molecule 28: 50S RIBOSOMAL PROTEIN L30

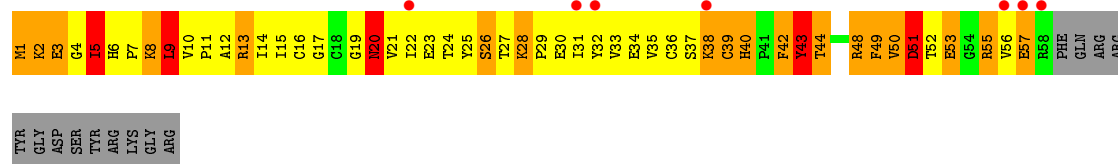


• Molecule 29: 50S RIBOSOMAL PROTEIN L31

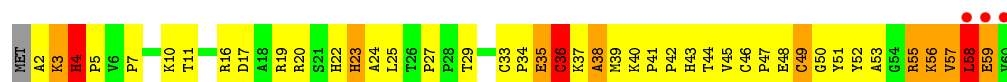




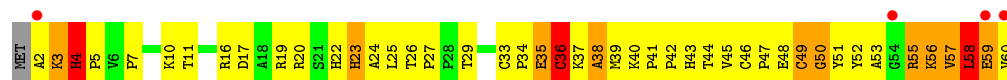
• Molecule 29: 50S RIBOSOMAL PROTEIN L31



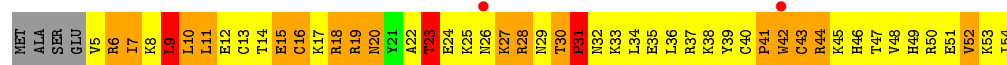
• Molecule 30: 50S RIBOSOMAL PROTEIN L32



• Molecule 30: 50S RIBOSOMAL PROTEIN L32



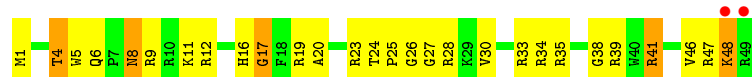
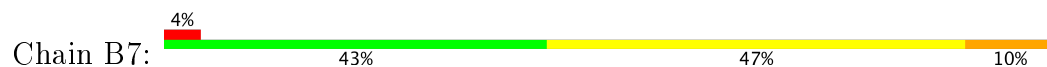
• Molecule 31: 50S RIBOSOMAL PROTEIN L33



• Molecule 31: 50S RIBOSOMAL PROTEIN L33



• Molecule 32: 50S RIBOSOMAL PROTEIN L34



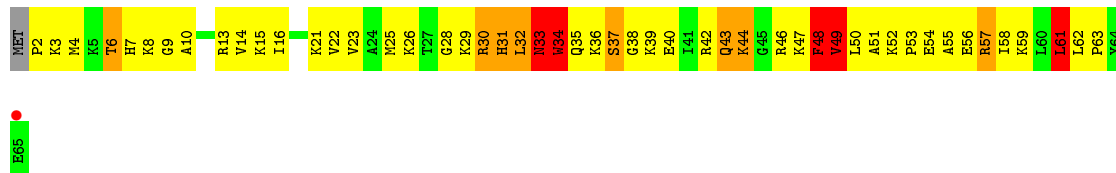
- Molecule 32: 50S RIBOSOMAL PROTEIN L34

Chain D7: 



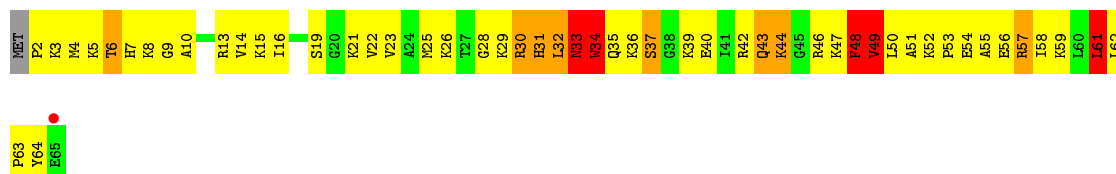
- Molecule 33: 50S RIBOSOMAL PROTEIN L35

Chain B8: 



- Molecule 33: 50S RIBOSOMAL PROTEIN L35

Chain D8: 



- Molecule 34: 50S RIBOSOMAL PROTEIN L36

Chain B9: 



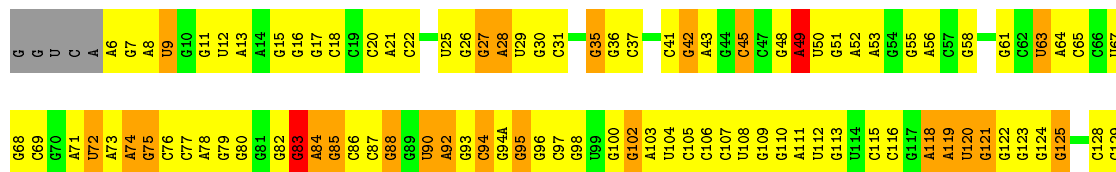
- Molecule 34: 50S RIBOSOMAL PROTEIN L36

Chain D9: 



- Molecule 35: 23S RIBOSOMAL RNA

Chain BA: 



|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|-------|-------|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| G1068 | A1069 | C1067 | G1071 | A1072 | A1073 | G1074 | C1075 | G1076 | A1077 | G1078 | G1079 | C1080 | U1081 | A1084 | A1088 | G1089 | U1090 | G1091 | G1092 | G1093 | U1094 | A1095 | A1096 | U1097 | A1098 | U1099 | G1100 | U1101 | C1102 | A1103 | G1104 | U1105 | G1106 | G1107 | U1108 | G1109 | G1110 | A1111 | G1112 | U1113 | G1114 | G1115 | G1116 | G1117 | C1118 | C1119 | G1120 | G1121 | G1122 | G1123 | G1124 | G1125 | A1126 | A1127 | A1128 | U1129 |       |       |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| G942  | U943  | G944  | A945  | G946  | G947  | G948  | G949  | G950  | G951  | G952  | A953  | G954  | C955  | U958  | A959  | A960  | C961  | G962  | U963  | G964  | C965  | G966  | G967  | G968  | U969  | C970  | C971  | G972  | A973  | G974  | C975  | G976  | C977  | G978  | G979  | G980  | U981  | U982  | U983  | U984  | U985  | U986  | U987  | U988  | U989  | U990  | C991  | C992  | G993  | U994  | A996  | G997  | C998  | U999  | A1000 | A1001 | C1002 | U1003 |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| U810  | U811  | C812  | U813  | C814  | C815  | C816  | C817  | C818  | A821  | U822  | G823  | A824  | C825  | U826  | U827  | U828  | A829  | G830  | G831  | G832  | U833  | C834  | A835  | G836  | C837  | C838  | U839  | C840  | A841  | G842  | G845  | G848  | A849  | C850  | U851  | G852  | C853  | G854  | G855  | C856  | C857  | U858  | G859  | U860  | A861  | G862  | A863  | G864  | C865  | A866  | G867  | U868  | G869  | A870  | U871  |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| C876  | U877  | A878  | G879  | G880  | G881  | G882  | G883  | G884  | C885  | C886  | A887  | C888  | C889  | A890  | G892  | C893  | C894  | U895  | G896  | C897  | A900  | A901  | C902  | C903  | C904  | U905  | G906  | U907  | C908  | A909  | A910  | C912  | U913  | C914  | C915  | G916  | A917  | A918  | C923  | G924  | C925  | A926  | G927  | G928  | U930  | G931  | G932  | A933  | C934  | C935  | C936  | U937  | G938  | G939  | A940  | U941  |       |       |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| G1005 | C1006 | C1007 | G1008 | A1009 | A1010 | C1011 | U1012 | G1013 | U1014 | G1015 | G1016 | U1019 | A1020 | G1021 | G1022 | U1023 | A1024 | G1025 | U1026 | A1027 | A1028 | A1029 | A1030 | U1033 | G1034 | U1035 | G1036 | G1037 | C1038 | G1039 | C1040 | C1041 | G1042 | U1043 | G1044 | A1045 | A1046 | G1047 | A1048 | U1049 | G1050 | G1051 | C1052 | C1053 | A1054 | U1057 | G1058 | G1059 | U1060 | G1061 | G1062 | U1063 | C1064 | A1067 |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| C134  | G135  | G136  | C137  | G139  | G139A | G140  | A141  | A142  | C142A | G143  | C143A | G145  | G146  | A149  | G152  | C153  | G154  | C154A | U155  | U156  | U157  | U158  | G171  | C172  | G173  | C174  | G175  | G176  | G177  | G178  | A182  | C183  | C184  | U185  | G186  | G187  | A190  | A191  | C192  | U193  | G194  | A195  | A196  | A197  | C198  | A199  | U200  | C201  | U202  | A203  | C204  | G205  | U206  |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| A207  | C208  | C209  | C210  | G211  | G212  | A213  | G214  | G215  | A216  | G217  | A218  | A221  | A222  | A223  | G226  | A227  | A228  | U229  | C230  | C231  | U234  | U235  | C238  | U239  | G240  | A241  | G242  | G245  | C246  | G247  | G248  | C249  | G250  | A251  | G252  | C253  | G254  | G259  | G260  | G261  | A265  | G266  | C267  | C268  | U269  | A270  | C271  | A271A | C271B | C271C | G271D | U271E |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| C271F | C271G | G271H | G271I | U271J | U271K | U271L | G271M | U271N | C271O | G271P | G271Q | G271R | G271S | G271T | G271U | G271V | U271Y | C271Z | G272  | U272A | G272B | G272C | G272D | C272G | C272H | U272I | C272J | G272K | G272L | G272M | G272N | G272O | G272P | G272Q | G272R | G272S | G272T | G272U | G272V | G272W | G272X | G272Y | G272Z | G273  | G274  | G275  | G276  | G277  | G278  | G279  | G280  | G281  | G282  | G283  | G284  | G285  | G286  | G287  | G288 | G289 | G290 | G291 | G292 | U293 | A294 | G295 | C296 | U299 | A270 | C271 | A271A | C271B | C271C | G271D | U271E |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| G304  | G307  | A310  | A311  | A320  | G321  | A322  | G323  | A324  | G325  | A326  | A327  | A328  | A329  | A330  | A331  | A332  | A333  | A334  | A335  | A336  | A337  | A338  | U339  | U339  | G340  | A341  | G342  | C343  | G344  | A345  | A346  | A347  | A348  | A422  | G349  | U350  | G351  | G352  | G353  | U358  | A359  | G360  | G361  | U362  | G363  | A363A | G363B | G363C | U363D | A443  | U363E | A363F | C364  | G365  | A371  | G372  | C373  | G374  | G375 | A376 | A377 | A378 | A379 | A380 | A381 | A382 | A383 | A384 | A385 | A386 | A387  | A388  | A389  | A390  | A391  | A392 | A393 | A394 | A395 | A396 | A397 | A398 | A399 | A400 | A401 | A402 | A403 | A404 | A405 | A406 | A407 | A408 | A409 | A410 | A411 | A412 | A413 | A414 | A415 | A416 | A417 | A418 | A419 | A420 | A421 | A422 | A423 | A424 | A425 | A426 | A427 | A428 | A429 | A430 | A431 | A432 | A433 | A434 | A435 | A436 | A437 | A438 | A439 | A440 | A441 | A442 | A443 | A444 | A445 | A446 | A447 | A448 | A449 | A450 | A451 | A452 | A453 | A454 | A455 | A456 | A457 | A458 | A459 | A460 | A461 | A462 | A463 | A464 | A465 | A466 | A467 | A468 | A469 | A470 | A471 | A472 | A473 | A474 | A475 | A476 | A477 | A478 | A479 | A480 | A481 | A482 | A483 | A484 | A485 | A486 | A487 | A488 | A489 | A490 | A491 | A492 | A493 | A494 | A495 | A496 | A497 | A498 | A499 | A500 | A501 | A502 | A503 | A504 | A505 | A506 | A507 | A508 | A509 | A510 | A511 | A512 | A513 | A514 | A515 |
| C516  | C517  | G518  | U519  | G520  | G521  | G522  | C523  | U524  | U525  | A526  | C527  | A528  | A529  | G530  | C531  | A532  | G533  | U534  | C535  | C536  | C537  | C538  | C539  | C540  | C541  | G544  | C545  | A547  | A548  | G549  | G551  | G552  | G553  | U554  | U555  | G556  | U557  | G558  | G559  | C560  | G561  | U562  | G563  | C564  | C565  | U566  | A567  | U568  | U569  | G570  | A571  | A572  | G573  | C574  | A575  | A576  | A577  | A578  | G579 |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| C580  | C581  | G582  | G583  | G584  | G585  | A586  | C587  | U588  | C589  | A590  | C591  | G592  | G593  | U594  | C595  | G598  | G599  | G600  | G601  | G602  | A603  | G604  | G605  | G606  | U607  | G608  | G609  | G610  | G611  | G612  | G613  | U614  | U614A | G614B | A614C | G615  | G616  | G618  | G619  | G620  | A621  | G622  | G623  | G624  | G625  | U626  | A627  | G628  | G629  | G630  | A631  | G634  | G635  | G636  | A637  | G638  | U639  |       |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| C640  | C641  | G642  | A643  | G644  | G645  | A646  | G647  | U648  | C649  | C650  | G651  | G652  | A653  | A654  | G654B | G654C | G654D | G654E | G654F | G654G | G654H | G654I | A654J | G654K | G654L | G654M | G654N | G654O | G654P | G654Q | G654R | G654S | G654T | A654U | A654V | A655  | G656  | G657  | G658  | G659  | G660  | G661  | G662  | G663  | G664  | G665  | G666  | U667  | G668  | G669  | G670  | G671  | G672  | G673  | G674  | G675  | A676  | A677  | A678 | A679 | A680 | A681 | A682 | A683 | A684 | A685 | A686 | A687 | A688 | A689 | A690  | A691  | A692  | A693  | A694  | A695 | A696 | A697 | A698 | A699 | A700 | A701 | A702 | A703 | A704 | A705 | A706 | A707 | G708 | G709 | G710 | G711 | A718 | G719 | G720 | G721 | A722 | G723 | G724 | G725 | G726 | A727 | G728 | G729 | G730 | G733 | G737 | G738 | G739 | G740 | G741 | G742 | G743 | G744 | G745 | A746 | U747 | G748 | G749 |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| A750  | A751  | A752  | C753  | C754  | C755  | C756  | U757  | G758  | U759  | G760  | A761  | U762  | G763  | G764  | G765  | G766  | G767  | G768  | G769  | G770  | G771  | G772  | U773  | A774  | G775  | G776  | A777  | G778  | U779  | G780  | A781  | A782  | A783  | A784  | G785  | G786  | U787  | A788  | G789  | C790  | G791  | G792  | G793  | G794  | C795  | C796  | C797  | U798  | A801  | G802  | A803  | A804  | G805  | C806  | U807  | G808  | G809  |       |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| U810  | U811  | C812  | U813  | C814  | C815  | C816  | C817  | C818  | A821  | U822  | G823  | A824  | C825  | U826  | U827  | U828  | A829  | G830  | G831  | G832  | U833  | C834  | A835  | G836  | C837  | C838  | U839  | C840  | A841  | G842  | G845  | G848  | A849  | C850  | U851  | G852  | C853  | G854  | G855  | C856  | C857  | U858  | G859  | U860  | A861  | G862  | A863  | G864  | C865  | A866  | G867  | U868  | G869  | A870  | U871  |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| C876  | U877  | A878  | G879  | G880  | G881  | G882  | G883  | G884  | C885  | C886  | A887  | C888  | C889  | A890  | G892  | C893  | C894  | U895  | G896  | C897  | A900  | A901  | C902  | C903  | C904  | U905  | G906  | U907  | C908  | A909  | A910  | C912  | U913  | C914  | C915  | G916  | A917  | A918  | C923  | G924  | C925  | A926  | G927  | G928  | U930  | G931  | G932  | A933  | C934  | C935  | C936  | U937  | G938  | G939  | A940  | U941  |       |       |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| G1005 | C1006 | C1007 | G1008 | A1009 | A1010 | C1011 | U1012 | G1013 | U1014 | G1015 | G1016 | U1019 | A1020 | G1021 | G1022 | U1023 | A1024 | G1025 | U1026 | A1027 | A1028 | A1029 | A1030 | U1033 | G1034 | U1035 | G1036 | G1037 | C1038 | G1039 | C1040 | C1041 | G1042 | U1043 | G1044 | A1045 | A1046 | G1047 | A1048 | U1049 | G1050 | G1051 | C1052 | C1053 | A1054 | U1057 | G1058 | G1059 | U1060 | G1061 | G1062 | U1063 | C1064 | A1067 |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |

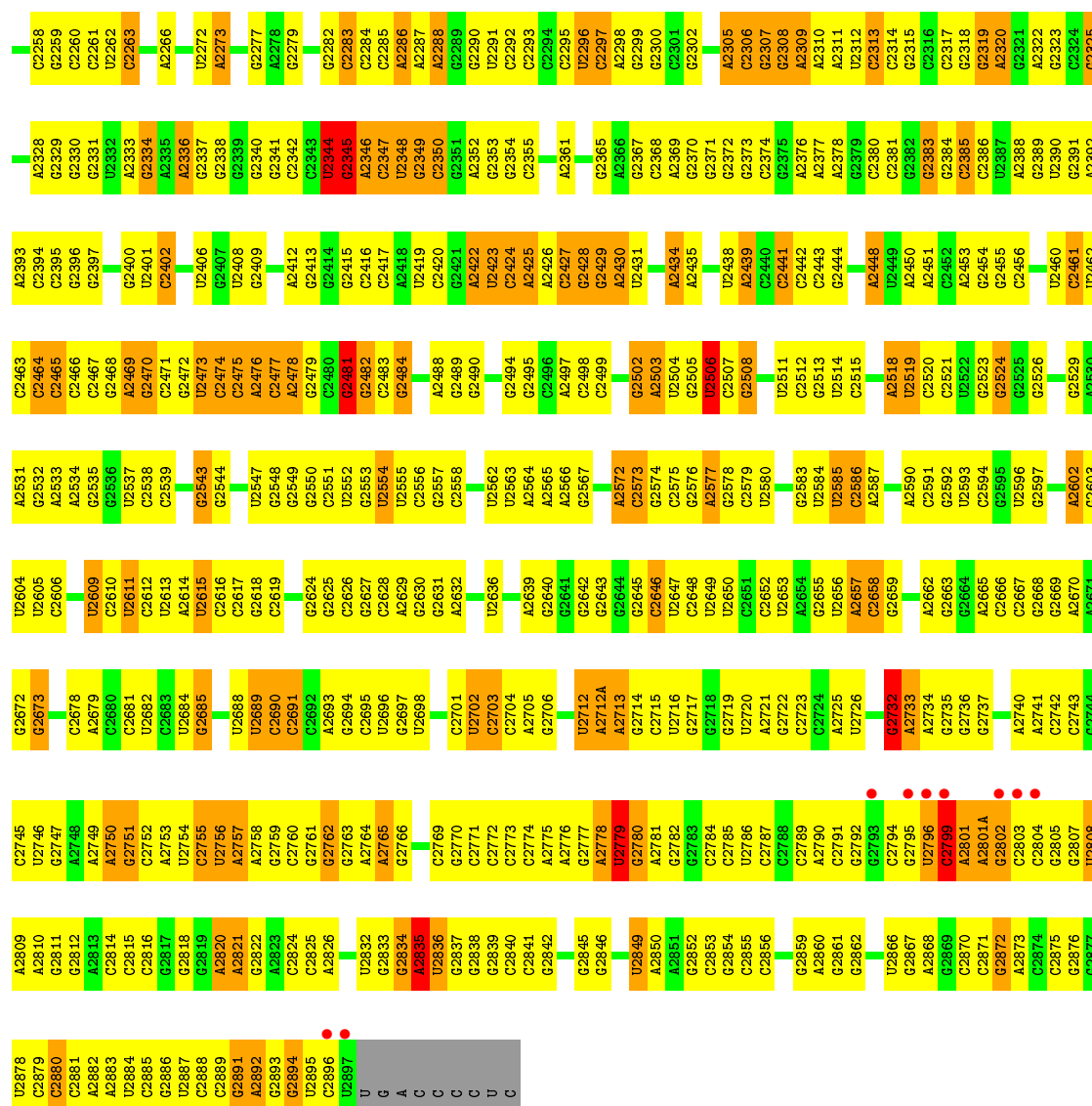
|       |       |       |       |       |       |       |        |        |        |        |        |
|-------|-------|-------|-------|-------|-------|-------|--------|--------|--------|--------|--------|
| G2046 | G1909 | G1830 | U1768 | G1675 | A1603 | G1537 | C1467  | U1397  | G1328  | G1258  | A1132  |
| G1983 | G1910 | G1831 | G1769 | A1676 | C1607 | G1538 | A1472  | C1398  | U1329  | G1259  | U1133  |
| G1984 | U1911 | G1832 | G1770 | A1677 | C1608 | G1539 | G1473  | C1399  | C1330  | G1260  | C1196  |
| G1985 | A1912 | U1833 | G1771 | G1678 | A1609 | U1540 | C1474  | G1401  | A1331  | C1261  | G1197  |
| A1986 | A1913 | G1834 | G1772 | U1679 | A1610 | G1541 | C1475  | C1402  | G1333  | U1262  | G1137  |
| G1987 | G1914 | G1835 | U1773 | U1680 | C1611 | A1542 | C1476  | C1403  | G1334  | G1263  | G1138  |
| G1988 | U1917 | G1838 | G1774 | G1681 | C1611 | C1543 | A1477  | C1404  | G1335  | A1265  | G1139  |
| G1989 | A1918 | G1839 | U1775 | G1682 | A1614 | A1544 | G1478  | U1405  | G1336  | U1205  | C1140  |
| G1990 | A1919 | G1840 | G1776 | C1683 | C1615 | A1545 | A1478  | U1406  | G1337  | U1267  | U1141  |
| U1993 | G1920 | U1841 | U1777 | C1684 | A1616 | C1546 | G1482  | C1407  | U1268  | U1142  | A1142A |
| G1996 | G1921 | G1842 | U1778 | U1688 | C1617 | C1551 | G1483  | C1408  | A1269  | G1209  | A1143  |
| G1997 | G1922 | C1843 | A1780 | A1689 | A1618 | G1552 | G1485  | C1409  | A1270  | A1210  | A1144  |
| G1998 | C1844 | C1782 | C1781 | U1692 | G1623 | A1553 | A1486  | G1410  | G1271  | U1211  | C1145  |
| G1999 | G1846 | U1783 | U1693 | U1692 | A1624 | A1554 | G1488  | C1411  | A1272  | G1212  | C1146  |
| G2000 | A1847 | A1784 | C1694 | C1694 | C1625 | A1555 | G1489  | U1415  | U1273  | A1213  | C1147  |
| G2001 | A1848 | A1785 | C1694 | C1694 | C1625 | A1556 | U1490  | G1416  | A1274  | G1215  | A1148  |
| G2002 | G1929 | U1786 | G1697 | U1629 | U1629 | A1557 | A1491  | C1417  | A1275  | G1216  | A1149  |
| G2003 | G1930 | A1787 | A1698 | G1630 | G1630 | A1558 | G1492  | U1420  | A1276  | C1217  | C1150  |
| G2004 | U1931 | C1850 | A1787 | G1630 | G1630 | G1559 | C1493  | U1421  | G1277  | C1218  | G1151  |
| G2005 | U1932 | U1851 | C1788 | A1632 | A1632 | G1560 | C1494  | G1421  | A1278  | G1219  | C1152  |
| G2006 | G1933 | A1852 | A1789 | A1633 | A1633 | G1561 | A1494  | A1495  | A1220  | A1220  | C1153  |
| G2007 | C1934 | A1853 | C1790 | A1634 | A1634 | G1562 | A1496  | A1496  | A1221  | G1154  | G1154  |
| G2008 | G1935 | A1854 | A1791 | A1635 | A1635 | G1563 | U1497  | A1497  | C1221A | C1221A | A1155  |
| G2009 | A1936 | G1855 | U1794 | A1636 | A1636 | C1564 | C1498  | G1429  | C1222  | C1222  | A1156  |
| G2010 | A1937 | G1856 | U1795 | A1637 | A1637 | A1566 | C1499  | U1430  | G1223  | G1223  | G1157  |
| G2011 | A1938 | G1857 | U1796 | A1638 | A1638 | A1567 | G1500  | U1431  | C1224  | C1224  | C1158  |
| G2012 | C1941 | A1858 | U1797 | A1639 | A1639 | G1568 | G1500  | C1432  | G1225  | G1225  | U1159  |
| G2013 | C1942 | A1859 | G1799 | A1640 | A1640 | A1569 | U1503  | U1433  | A1226  | A1226  | G1160  |
| G2014 | U1943 | G1862 | C1800 | A1641 | A1641 | A1570 | C1504  | U1434  | G1227  | G1227  | C1161  |
| G2015 | U1944 | G1863 | G1801 | C1644 | C1644 | A1571 | C1505  | G1435  | G1228  | G1228  | G1162  |
| G2016 | U1945 | U1864 | G1802 | G1645 | G1645 | A1572 | C1506  | G1436  | G1229  | G1229  | G1163  |
| G2017 | U1946 | G1865 | A1803 | G1646 | G1646 | A1573 | C1509  | U1437  | U1165  | U1165  | U1165  |
| G2018 | C1947 | G1866 | A1804 | G1647 | G1647 | C1574 | A1509A | C1438  | G1231  | G1231  | C1166  |
| G2019 | U1948 | C1867 | U1805 | G1648 | G1648 | A1575 | A1509B | A1439  | G1232  | G1232  | C1167  |
| G2020 | G1949 | A1877 | C1806 | G1649 | G1649 | U1576 | G1510  | G1440  | C1233  | C1233  | U1167  |
| G2021 | G1950 | G1878 | G1807 | G1650 | G1650 | C1577 | G1511  | G1441  | U1234  | U1234  | G1168  |
| G2022 | U1951 | C1882 | U1808 | G1651 | G1651 | U1578 | U1512  | G1442  | G1235  | G1235  | G1169  |
| G2023 | A1952 | G1883 | A1809 | A1654 | A1654 | A1579 | C1513  | U1514  | G1236  | G1236  | G1170  |
| G2024 | G1953 | A1884 | A1810 | A1655 | A1655 | C1582 | U1514  | C1445A | G1237  | G1237  | G1171  |
| G2025 | U1954 | A1885 | A1812 | C1656 | C1656 | A1583 | G1515  | C1446  | G1238  | G1238  | A1174  |
| G2026 | U1955 | C1886 | A1813 | C1657 | C1657 | A1584 | C1516  | G1447  | U1240  | U1240  | U1175  |
| G2027 | U1956 | C1887 | G1814 | C1658 | C1658 | A1587 | G1517  | G1448  | A1241  | A1241  | G1176  |
| G2028 | U1957 | G1888 | A1815 | U1659 | U1659 | A1588 | U1523  | C1450A | A1242  | A1242  | A1177  |
| G2029 | C1958 | A1889 | G1816 | C1660 | C1660 | C1589 | G1524  | C1451  | G1243  | G1243  | C1180  |
| G2030 | A1959 | G1891 | G1817 | G1661 | G1661 | U1590 | G1525  | A1452  | C1314  | C1314  | C1181  |
| A1960 | U1960 | C1892 | U1818 | G1662 | G1662 | G1591 | G1526  | U1453  | G1315  | A1245  | A1182  |
| U1963 | U1963 | C1892 | U1819 | C1663 | C1663 | G1592 | G1527  | G1455  | G1316  | A1246  | A1183  |
| G1964 | G1964 | G1899 | U1820 | A1664 | A1664 | G1594 | A1528  | G1459  | A1317  | G1248  | G1184  |
| G1967 | C1967 | A1900 | G1821 | A1665 | A1665 | G1595 | A1528A | G1460  | C1318  | U1249  | C1185  |
| G1968 | G1968 | A1901 | G1822 | G1666 | G1666 | A1596 | G1529  | G1461  | G1319  | G1250  | G1186  |
| G1969 | A1969 | C1902 | G1824 | G1667 | G1667 | A1597 | U1530  | C1462  | G1387  | G1251  | G1187  |
| A1970 | G1970 | G1903 | G1825 | A1668 | A1668 | C1598 | C1531  | C1463  | U1323  | G1252  | U1188  |
| A1971 | A1971 | G1906 | G1826 | A1669 | A1669 | C1599 | U1534  | C1464  | A1322  | G1253  | A1189  |
| A1972 | G1972 | G1907 | C1827 | C1670 | C1670 | C1600 | U1535  | G1465  | G1324  | A1254  | G1190  |
| C2043 | C1974 | C1908 | A1829 | G1674 | G1674 | U1602 | C1536  | G1466  | G1325  | U1255  | G1191  |
|       |       |       |       |       |       |       |        |        | U1326  | G1256  | G1192  |
|       |       |       |       |       |       |       |        |        | C1327  | C1257  | G1193  |
| G2115 | G2046 | G1983 | U1768 | G1675 | A1603 | G1537 | C1467  | U1397  | G1328  | G1258  | A1132  |
| G2116 | G2050 | G1984 | G1770 | A1677 | C1607 | G1538 | A1472  | C1398  | U1329  | G1259  | U1133  |
| A2117 | A2051 | G1985 | G1771 | G1678 | A1608 | G1539 | G1473  | C1399  | C1330  | G1260  | C1196  |
| G2118 | G2052 | A1986 | G1772 | U1679 | A1609 | U1540 | C1474  | G1401  | A1331  | C1261  | G1197  |
| G2119 | G2053 | G1987 | U1773 | U1680 | A1610 | G1541 | C1475  | C1402  | G1333  | U1262  | G1137  |
| G2120 | G2054 | G1988 | G1774 | G1681 | C1611 | A1542 | C1476  | C1403  | G1334  | G1263  | G1138  |
| G2121 | G2055 | G1989 | U1775 | G1682 | C1611 | C1543 | A1477  | C1404  | G1335  | A1265  | G1139  |
| U2122 | G2056 | U1990 | G1776 | C1683 | A1614 | A1544 | G1478  | U1405  | G1336  | U1205  | C1140  |
| G2123 | A2057 | U1991 | U1777 | C1684 | C1615 | A1545 | A1478  | U1406  | G1337  | U1267  | U1141  |
| A2126 | G2058 | U1992 | U1778 | U1688 | C1617 | C1551 | G1482  | C1407  | U1268  | U1142  | A1142A |
| G2127 | A2059 | U1993 | U1779 | A1689 | A1618 | G1552 | G1483  | C1408  | A1269  | G1209  | A1143  |
| G2128 | A2060 | C1984 | A1780 | A1689 | A1618 | G1553 | G1485  | C1409  | A1270  | A1210  | A1144  |
| G2129 | G2061 | C1984 | C1781 | U1692 | G1623 | A1553 | A1486  | G1410  | G1271  | U1211  | C1145  |
| U2130 | A2062 | G1985 | U1693 | U1692 | A1624 | A1554 | G1488  | C1411  | A1272  | G1212  | C1146  |
| U2131 | G2063 | G1986 | C1782 | C1694 | C1625 | A1555 | G1489  | U1415  | U1273  | A1213  | C1147  |
| U2132 | G2064 | A1847 | A1784 | C1694 | C1625 | A1556 | U1490  | G1416  | A1274  | G1215  | A1148  |
| G2133 | G2065 | A1848 | A1785 | C1694 | C1625 | A1557 | A1491  | C1417  | A1275  | G1216  | A1149  |
| G2134 | G2066 | G1987 | U1786 | G1697 | U1629 | A1558 | G1492  | U1420  | A1276  | C1217  | C1150  |
| A2135 | G2067 | G1988 | A1787 | A1698 | G1630 | G1559 | C1493  | U1421  | G1277  | C1218  | G1151  |
| A2136 | U2068 | C1850 | A1787 | G1630 | G1630 | G1560 | C1494  | G1421  | A1278  | G1219  | C1152  |
| C2137 | G2069 | U1851 | C1788 | A1632 | A1632 | G1561 | A1494  | A1495  | A1220  | A1220  | C1153  |
| G2138 | G2070 | A1852 | A1789 | A1633 | A1633 | G1562 | A1496  | A1496  | A1221  | G1154  | G1154  |
| G2139 | A2071 | A1853 | C1790 | A1634 | A1634 | G1563 | U1497  | A1497  | C1221A | C1221A | A1155  |
| G2140 | G2072 | G1854 | A1791 | A1635 | A1635 | C1564 | C1498  | G1429  | C1222  | C1222  | A1156  |
| G2141 | G2073 | G1855 | U1794 | A1636 | A1636 | A1566 | C1499  | U1430  | G1223  | G1223  | G1157  |
| G2142 | U2074 | G1856 | U1795 | A1637 | A1637 | A1567 | G1500  | U1431  | C1224  | C1224  | C1158  |
| C2143 | U2075 | G1857 | U1796 | A1638 | A1638 | G1568 | G1500  | C1432  | G1225  | G1225  | U1159  |
| C2144 | U2076 | G1858 | U1797 | A1639 | A1639 | A1569 | U1503  | U1433  | A1226  | A1226  | G1160  |
| A2077 | G2077 | A1859 | G1799 | A1640 | A1640 | A1570 | C1504  | U1434  | G1227  | G1227  | C1161  |
| G2146 | G2078 | C1862 | C1800 | A1641 | A1641 | A1571 | C1505  | G1435  | G1228  | G1228  | G1162  |
| G2147 | U2079 | G1863 | G1801 | C1644 | C1644 | A1572 | C1506  | G1436  | G1229  | G1229  | G1163  |
| G2148 | G2080 | U1864 | G1802 | G1645 | G1645 | A1573 | C1509  | U1437  | U1165  | U1165  | U1165  |
| G2149 | C2081 | G1865 | A1803 | G1646 | G1646 | C1574 | A1509A | C1438  | G1231  | G1231  | C1166  |
| U2150 | A2082 | G1866 | A1804 | G1647 | G1647 | A1575 | A1509B | A1439  | G1232  | G1232  | C1167  |
| G2151 | G2083 | C1867 | U1805 | G1648 | G1648 | U1576 | G1510  | G1440  | C1233  | C1233  | U1167  |
| G2152 | U2084 | A1877 | C1806 | G1649 | G1649 | C1577 | G1511  | G1441  | U1234  | U1234  | G1168  |
| G2153 | G2085 | G1878 | G1807 | G1650 | G1650 | U1578 | U1512  | G1442  | G1235  | G1235  | G1169  |
| G2154 | G2086 | C1882 | U1808 | G1651 | G1651 | A1579 | C1513  | U1514  | G1236  | G1236  | G1170  |
| G2155 | U2087 | G1883 | A1809 | A1654 | A1654 | C1582 | U1514  | C1445A | G1237  | G1237  | G1171  |
| G2156 | G2088 | A1884 | A1810 | A1655 | A1655 | A1583 | G1515  | C1446  | G1238  | G1238  | A1174  |
| G2157 | U2091 | A1885 | A1812 | C1656 | C1656 | A1584 | C1516  | G1447  | U1240  | U1240  | U1175  |
| A2158 | U2092 | C1886 | A1813 | C1657 | C1657 | A1587 | G1517  | G1448  | A1241  | A1241  | G1176  |
| G2159 | G2093 | G1887 | G1814 | C1658 | C1658 | A1588 | U1523  | C1450A | A1242  | A1242  | A1177  |
| G2160 | G2094 | A1888 | A1815 | U1659 | U1659 | C1589 | G1524  | C1451  | G1243  | G1243  | C1180  |
| G2161 | C2097 | A1889 | G1816 | C1660 | C1660 | U1590 | G1525  | A1452  | C1314  | C1314  | C1181  |
| G2162 | U2098 | G1891 | G1817 | G1661 | G1661 | G1591 | G1526  | U1453  | G1315  | A1245  | A1182  |
| C2163 | G2100 | C1892 | U1818 | G1662 | G1662 | G1592 | G1527  | G1455  | G1316  | A1246  | A1183  |
| C2164 | U2103 | G1899 | U1820 | A1664 | A1664 | G1594 | A1528  | G1459  | A1317  | G1248  | G1184  |
| U2167 | G2104 | A1900 | G1821 | A1665 | A1665 | G1595 | A1528A | G1460  | C1318  | U1249  | C1185  |
| G2168 | A2105 | A1901 | G1822 | G1666 |       |       |        |        |        |        |        |



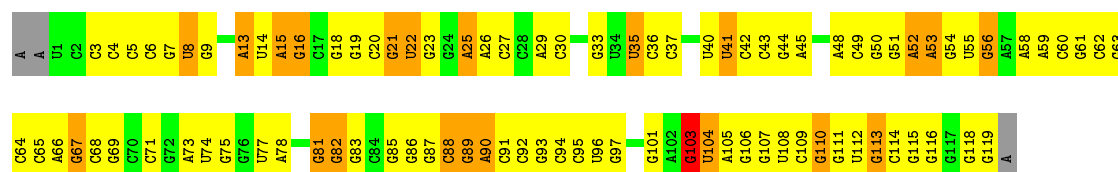




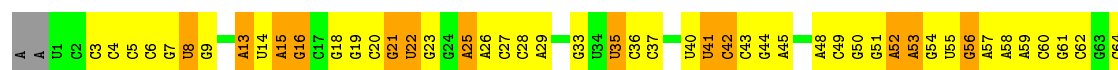


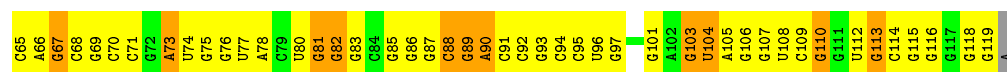


Chain BB: 22% 57% 17% ..

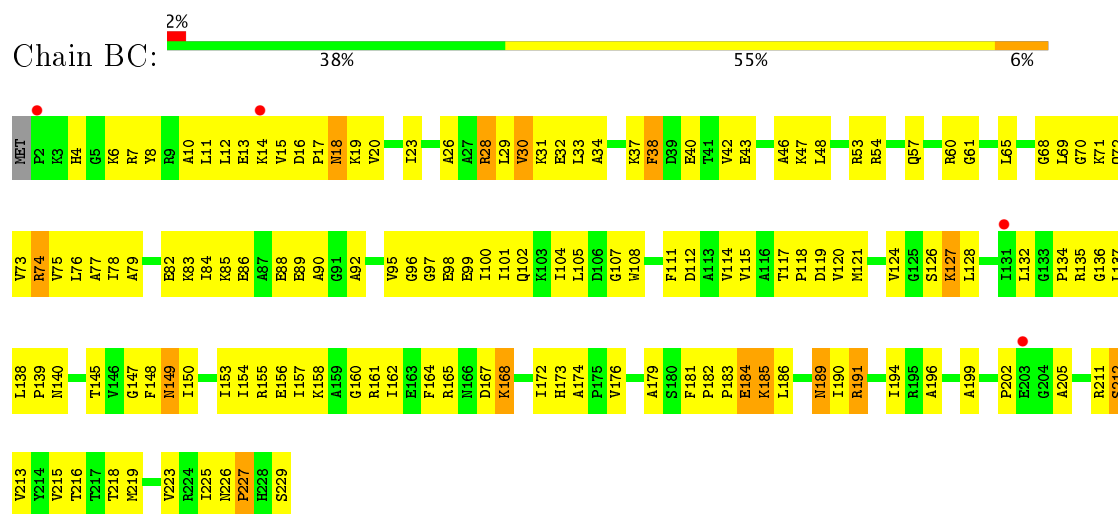


Chain DB: 20% 57% 20% .

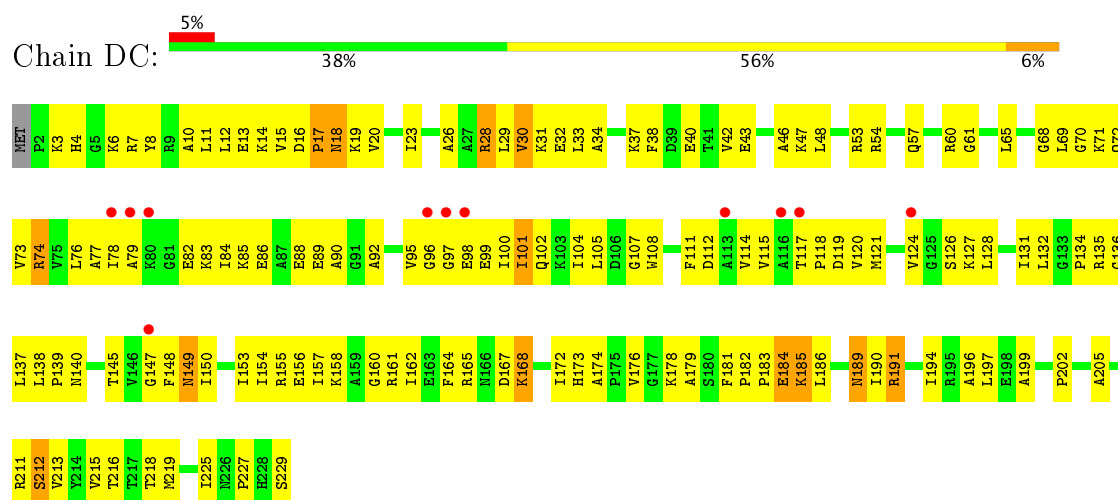




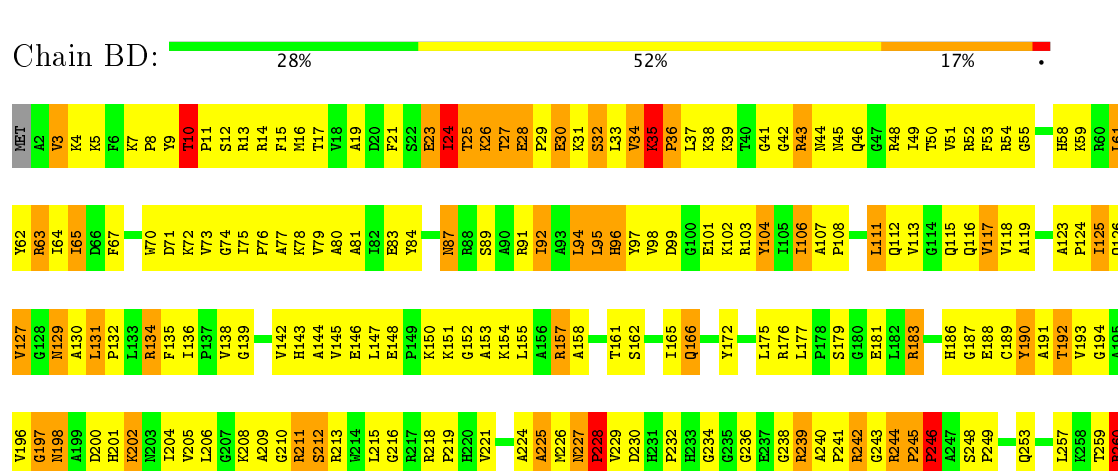
• Molecule 37: 50S RIBOSOMAL PROTEIN L1

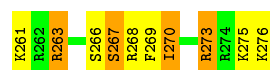


• Molecule 37: 50S RIBOSOMAL PROTEIN L1



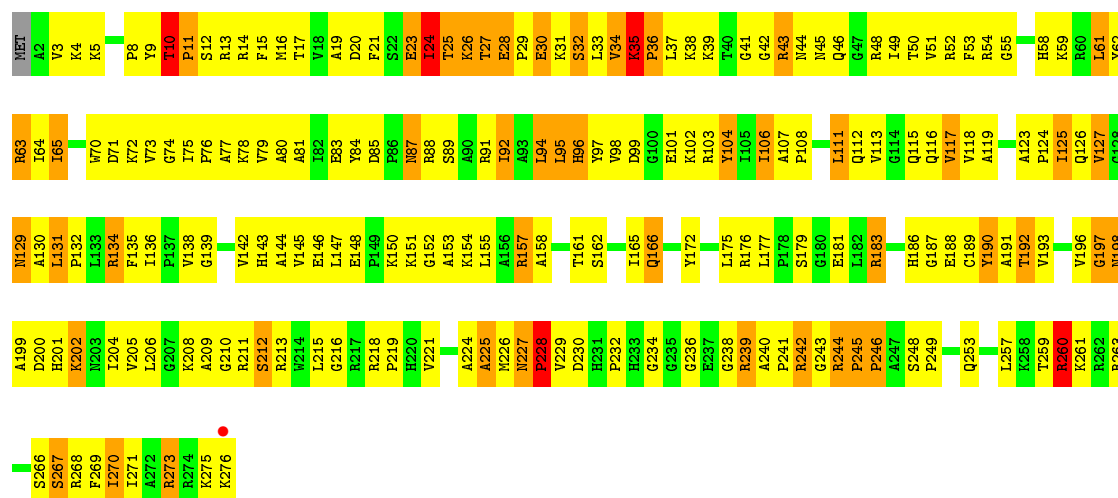
• Molecule 38: 50S RIBOSOMAL PROTEIN L2





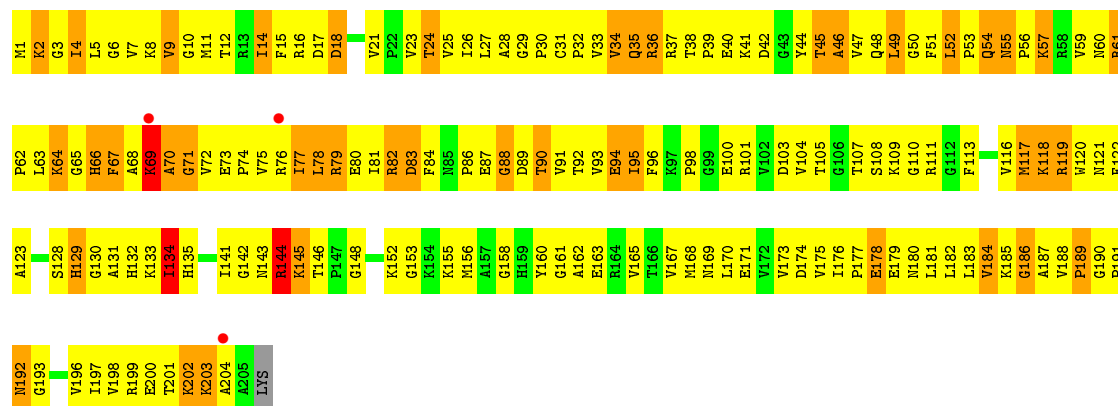
• Molecule 38: 50S RIBOSOMAL PROTEIN L2

Chain DD: 27% 54% 17%



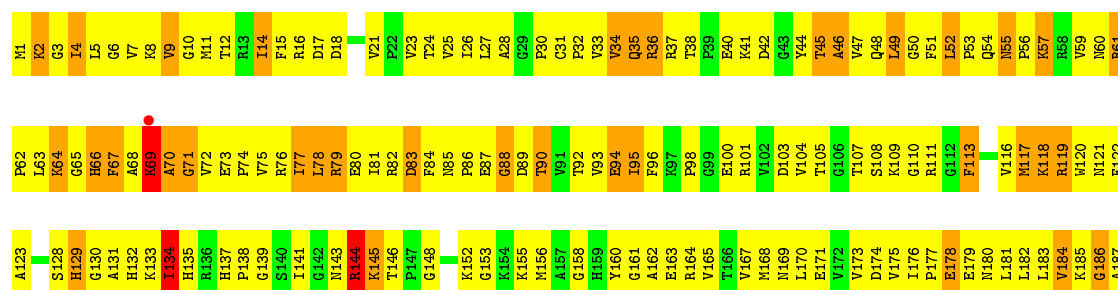
• Molecule 39: 50S RIBOSOMAL PROTEIN L3

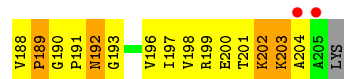
Chain BE: 17% 60% 21%



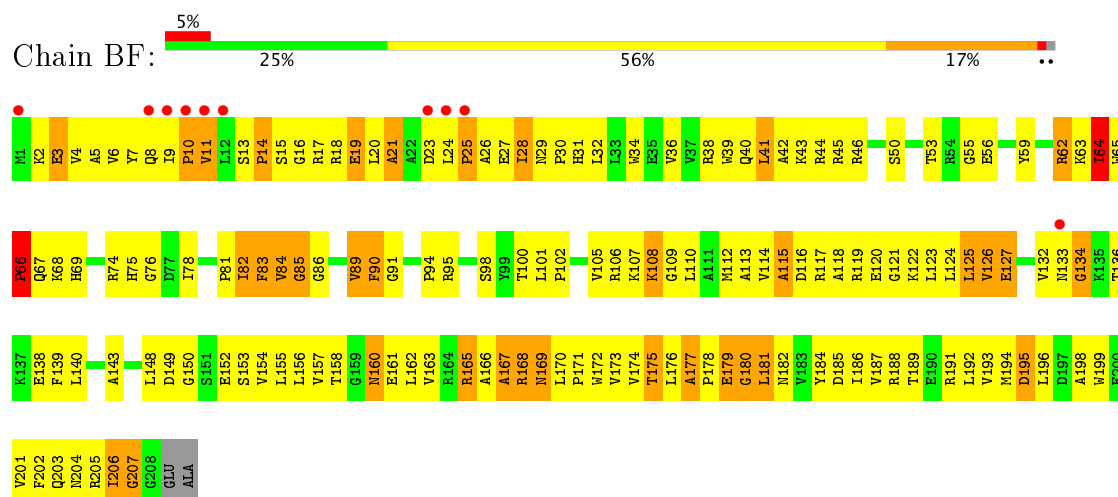
• Molecule 39: 50S RIBOSOMAL PROTEIN L3

Chain DE: 17% 62% 19%

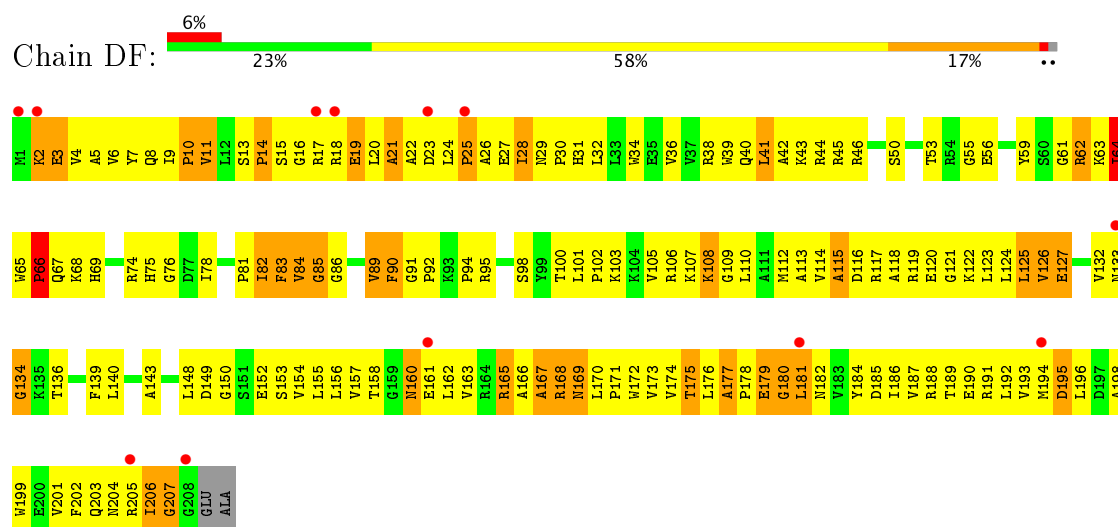




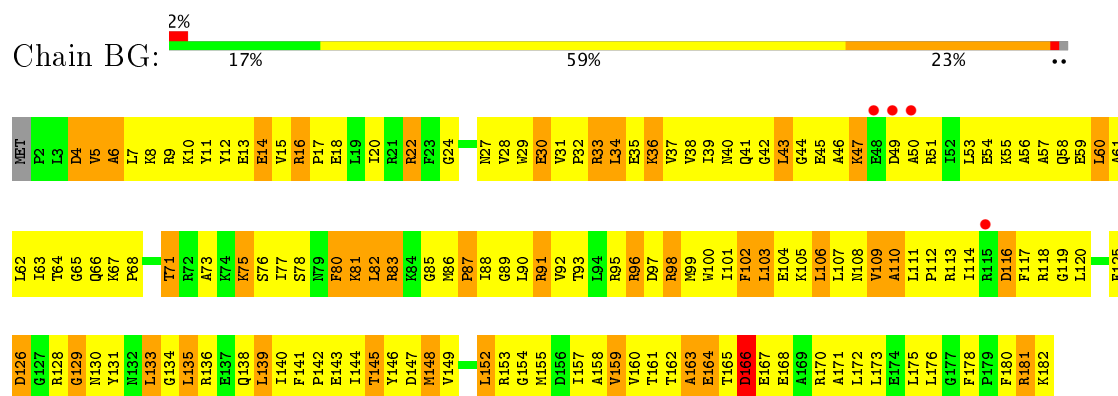
• Molecule 40: 50S RIBOSOMAL PROTEIN L4



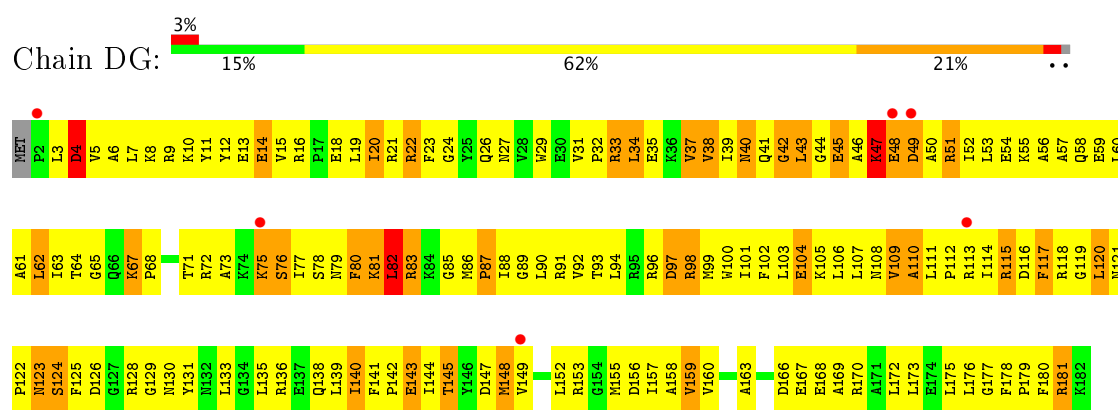
• Molecule 40: 50S RIBOSOMAL PROTEIN L4



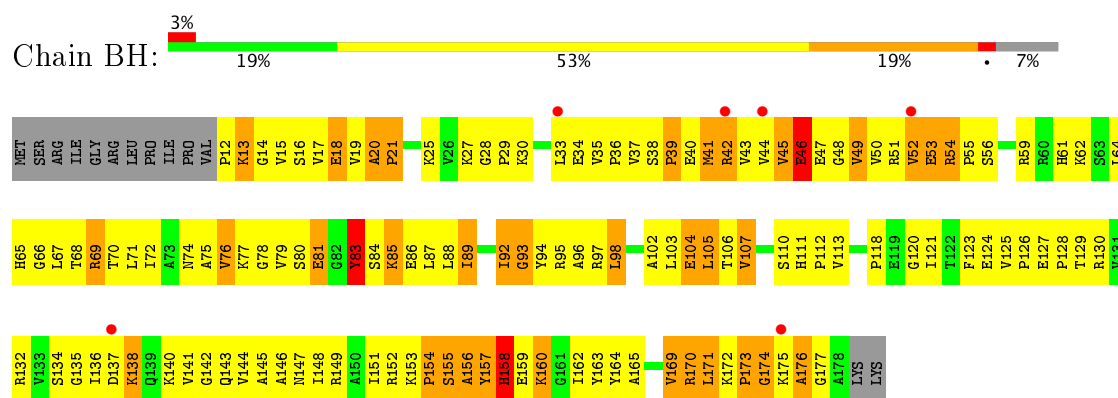
• Molecule 41: 50S RIBOSOMAL PROTEIN L5



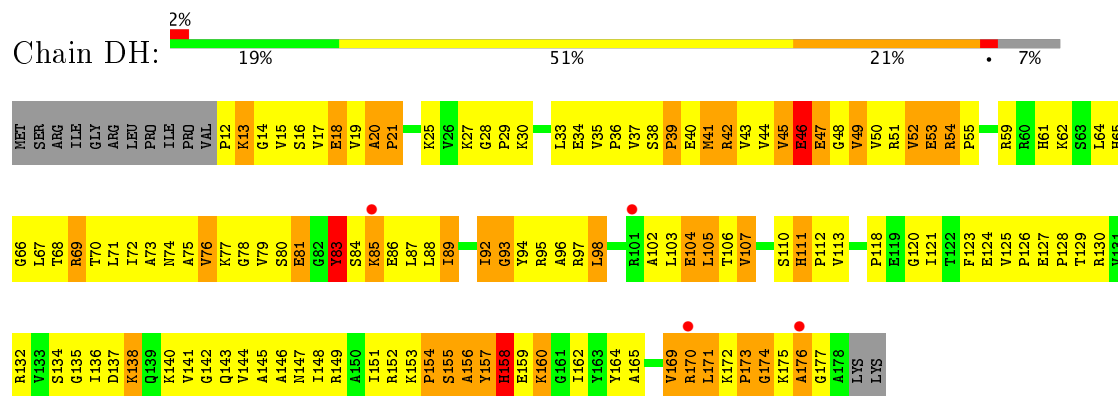
• Molecule 41: 50S RIBOSOMAL PROTEIN L5



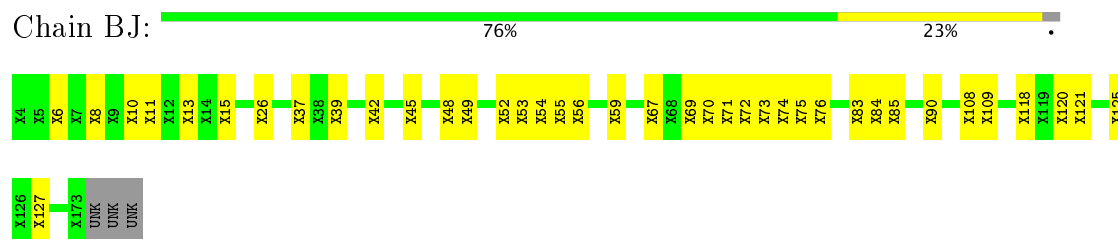
• Molecule 42: 50S RIBOSOMAL PROTEIN L6



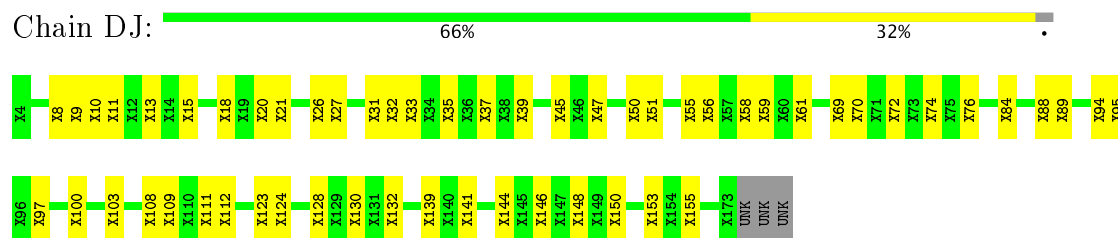
• Molecule 42: 50S RIBOSOMAL PROTEIN L6



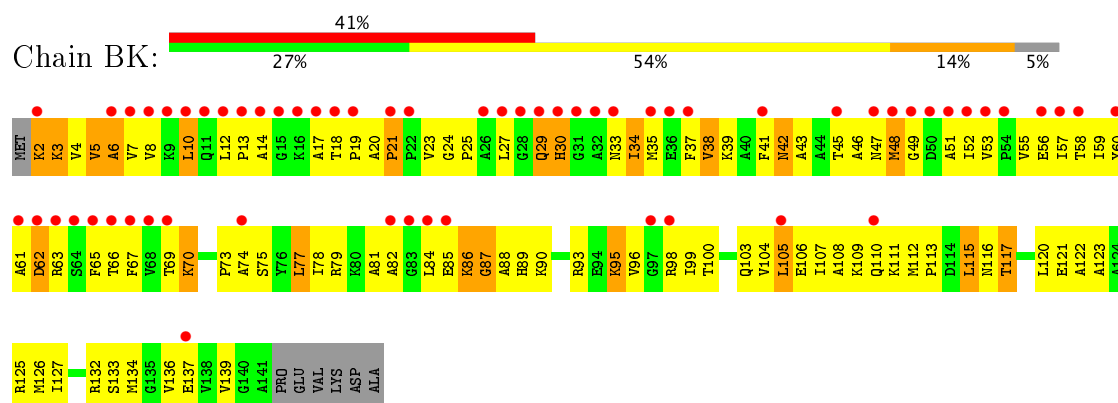
• Molecule 43: 50S RIBOSOMAL PROTEIN L10



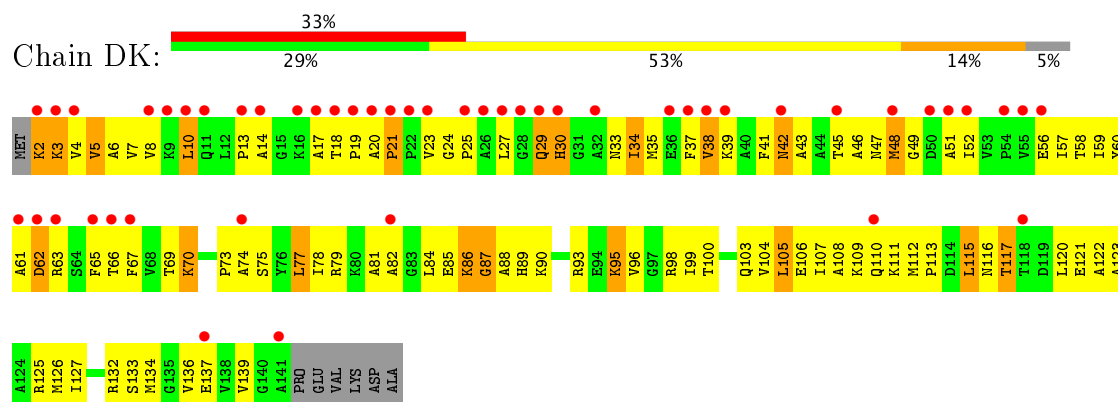
• Molecule 43: 50S RIBOSOMAL PROTEIN L10



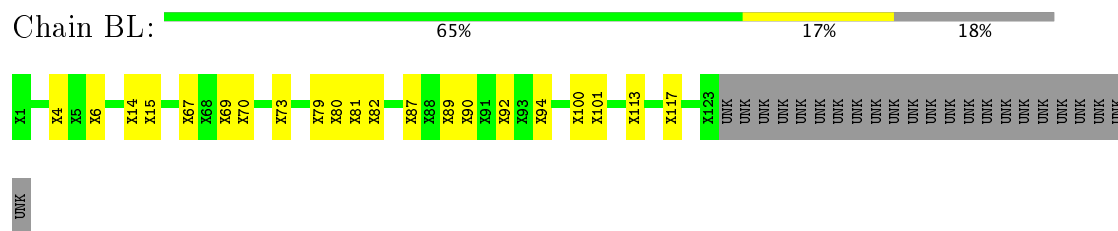
## ● Molecule 44: 50S RIBOSOMAL PROTEIN L11



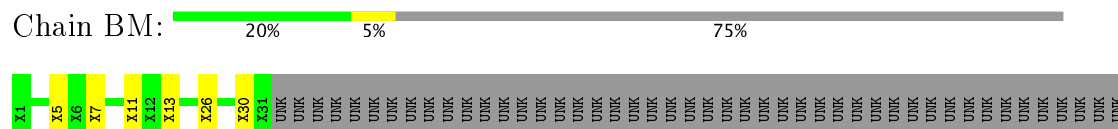
## ● Molecule 44: 50S RIBOSOMAL PROTEIN L11



## ● Molecule 45: 50S RIBOSOMAL PROTEIN L12



## ● Molecule 45: 50S RIBOSOMAL PROTEIN L12



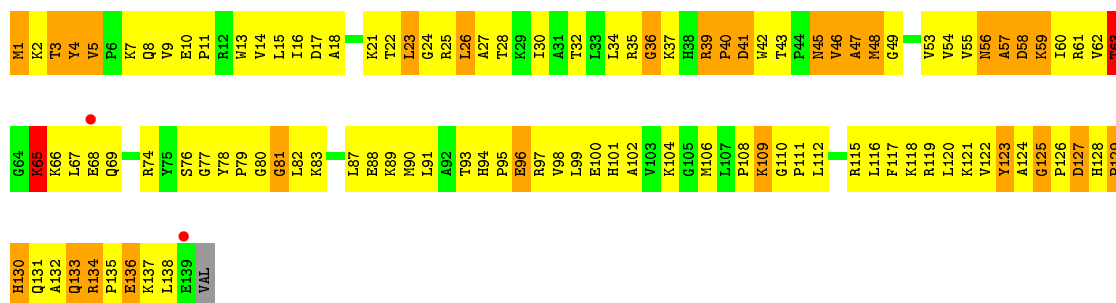


Chain Dm:  24% 76%



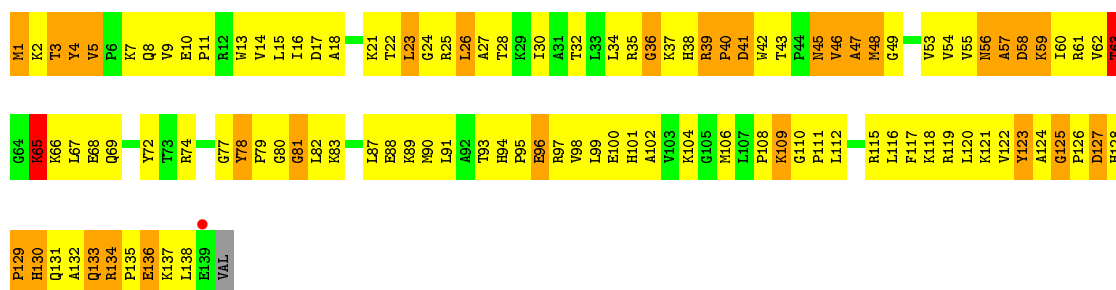
- Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain BN:  %



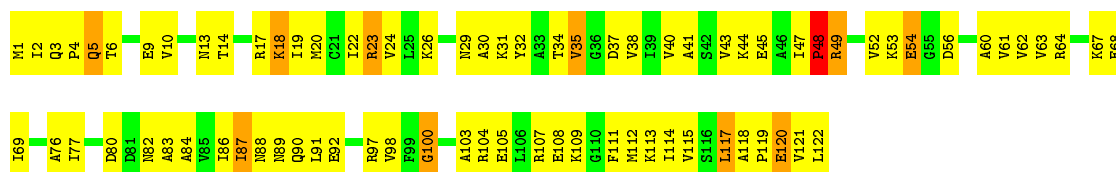
- Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain DN: 

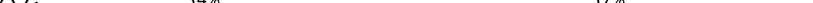


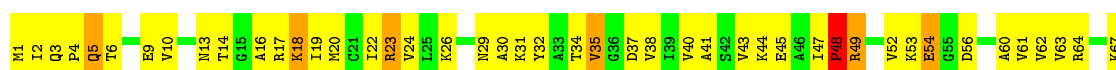
● Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain BO: 



- Molecule 47: 50S RIBOSOMAL PROTEIN L14

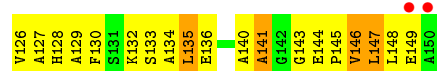
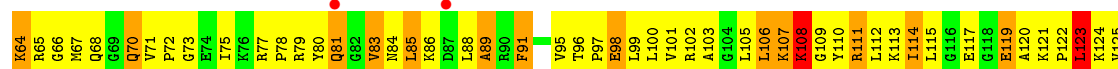
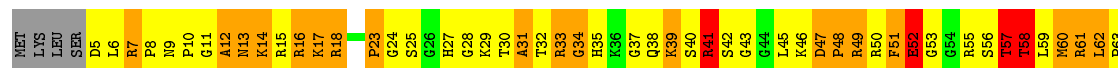
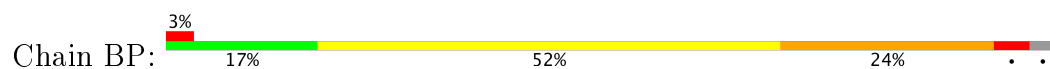
Chain DO: 



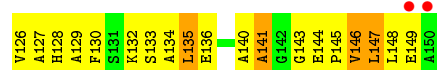
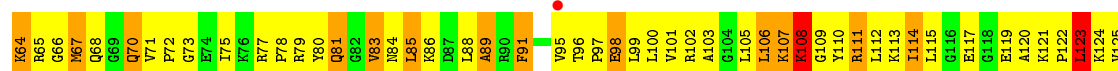
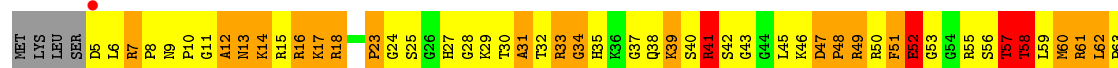
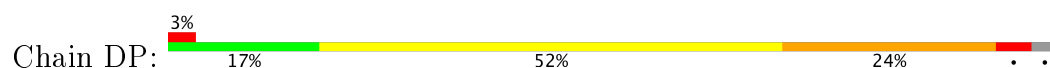




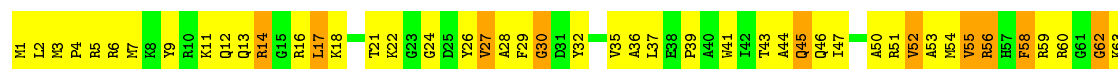
• Molecule 48: 50S RIBOSOMAL PROTEIN L15



• Molecule 48: 50S RIBOSOMAL PROTEIN L15

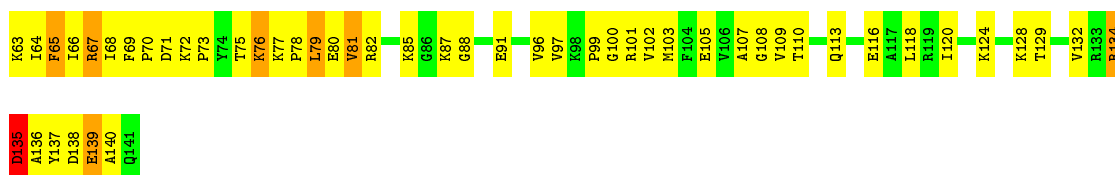


• Molecule 49: 50S RIBOSOMAL PROTEIN L16

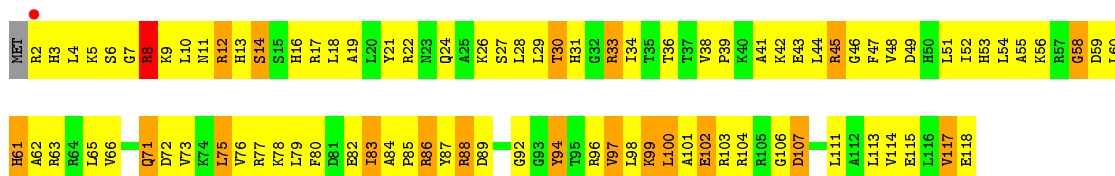


• Molecule 49: 50S RIBOSOMAL PROTEIN L16

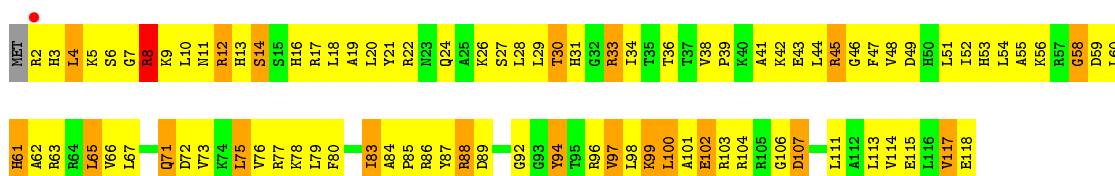




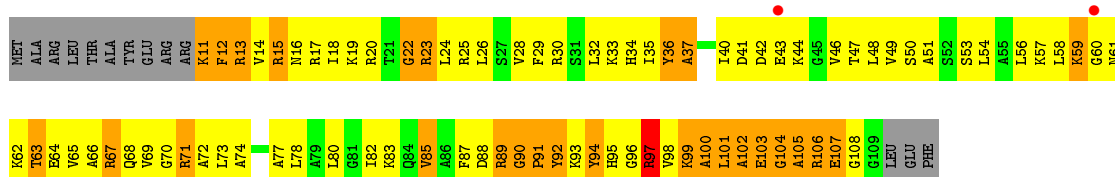
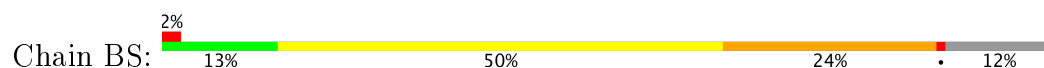
• Molecule 50: 50S RIBOSOMAL PROTEIN L17



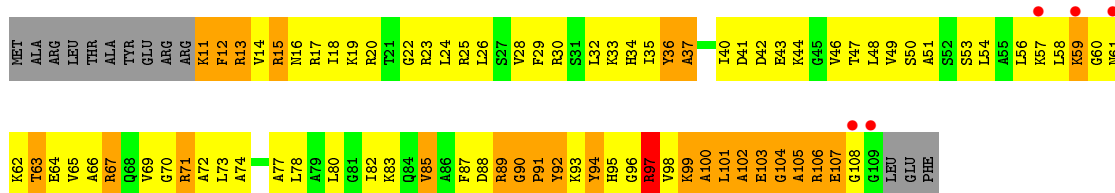
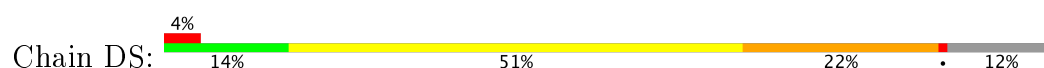
• Molecule 50: 50S RIBOSOMAL PROTEIN L17



• Molecule 51: 50S RIBOSOMAL PROTEIN L18

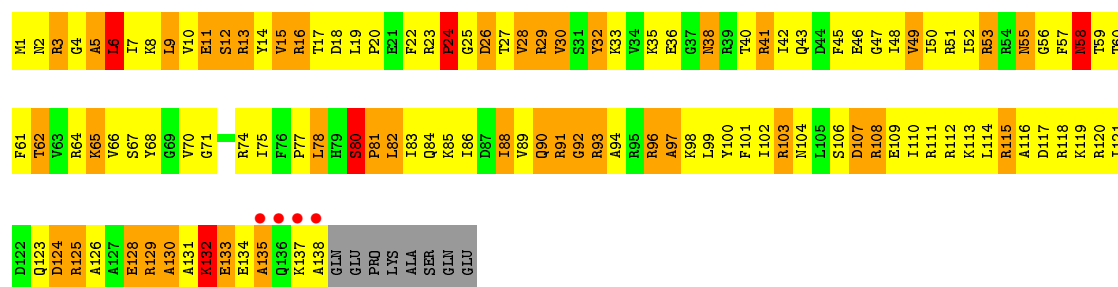


• Molecule 51: 50S RIBOSOMAL PROTEIN L18

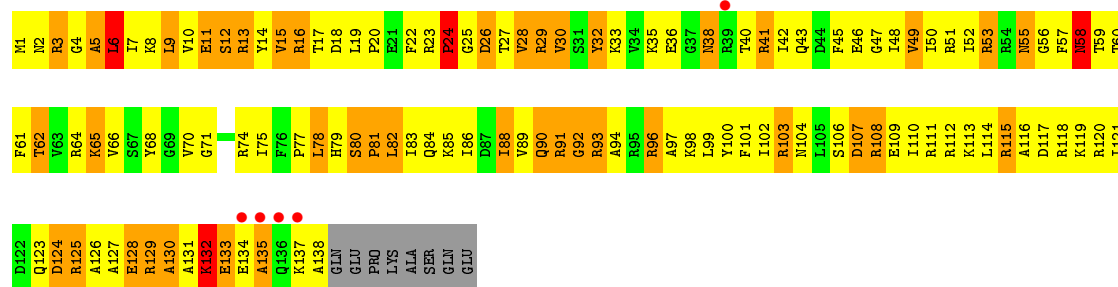
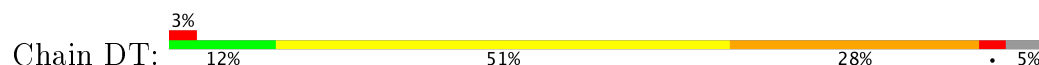


• Molecule 52: 50S RIBOSOMAL PROTEIN L19

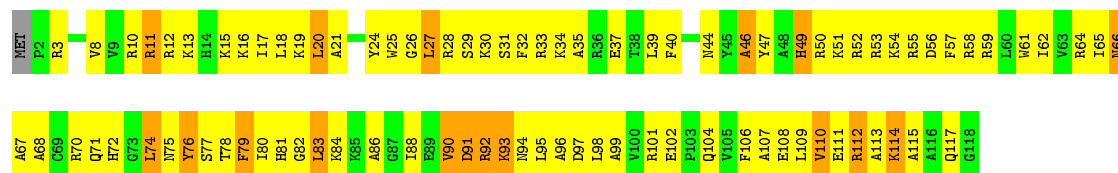




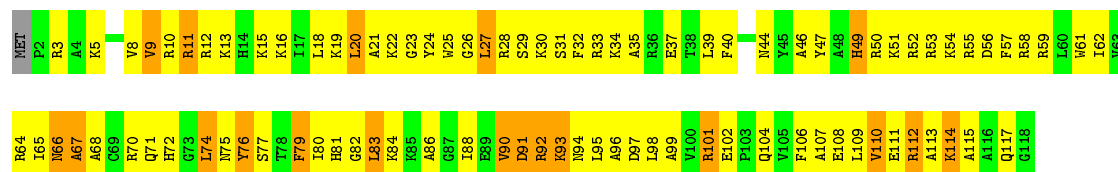
• Molecule 52: 50S RIBOSOMAL PROTEIN L19



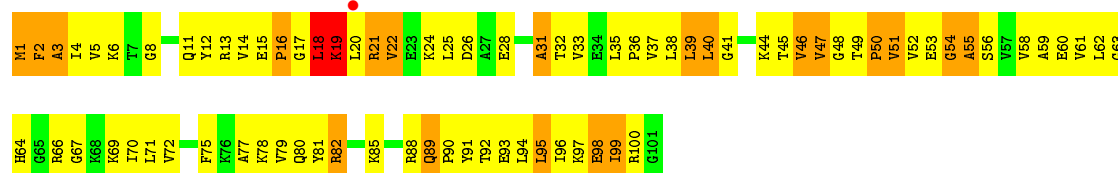
• Molecule 53: 50S RIBOSOMAL PROTEIN L20



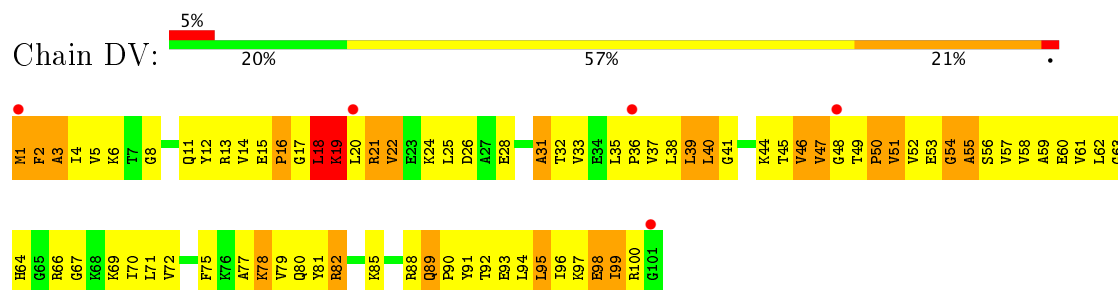
• Molecule 53: 50S RIBOSOMAL PROTEIN L20



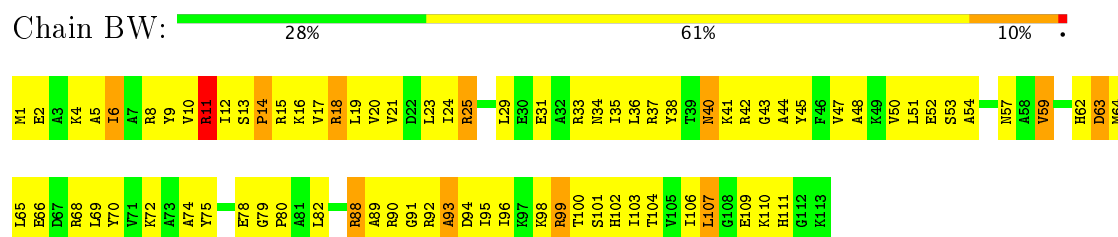
• Molecule 54: 50S RIBOSOMAL PROTEIN L21



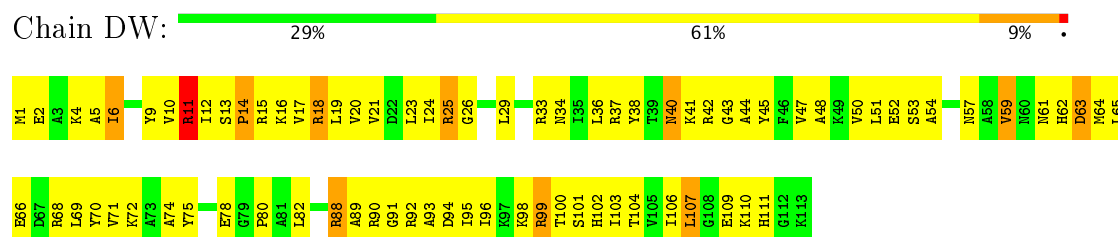
- Molecule 54: 50S RIBOSOMAL PROTEIN L21



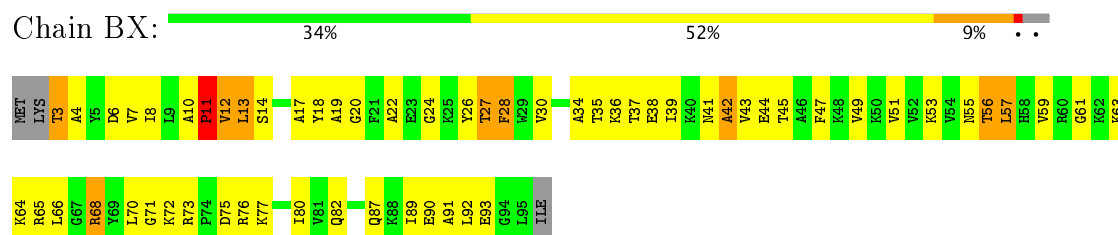
- Molecule 55: 50S RIBOSOMAL PROTEIN L22



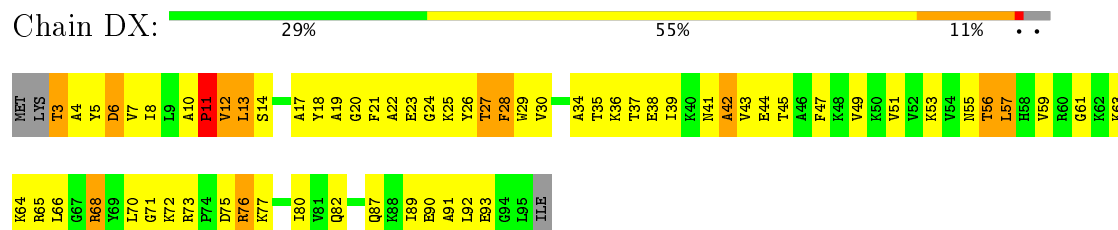
- Molecule 55: 50S RIBOSOMAL PROTEIN L22



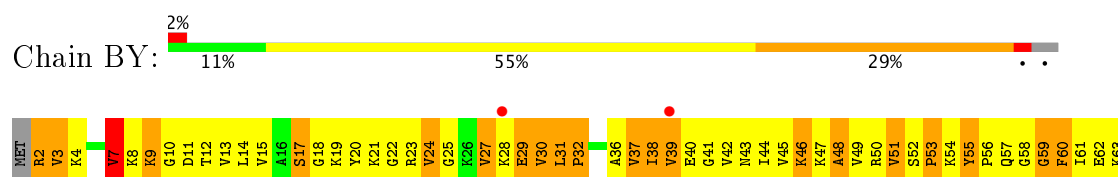
- Molecule 56: 50S RIBOSOMAL PROTEIN L23



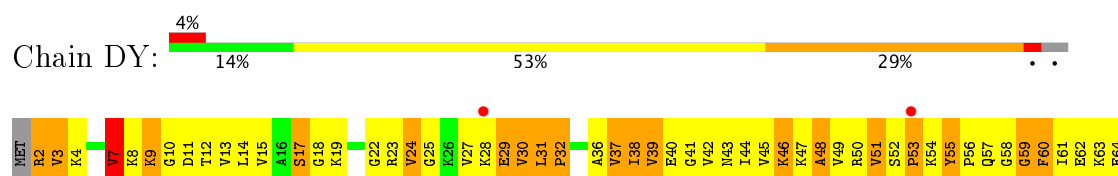
- Molecule 56: 50S RIBOSOMAL PROTEIN L23



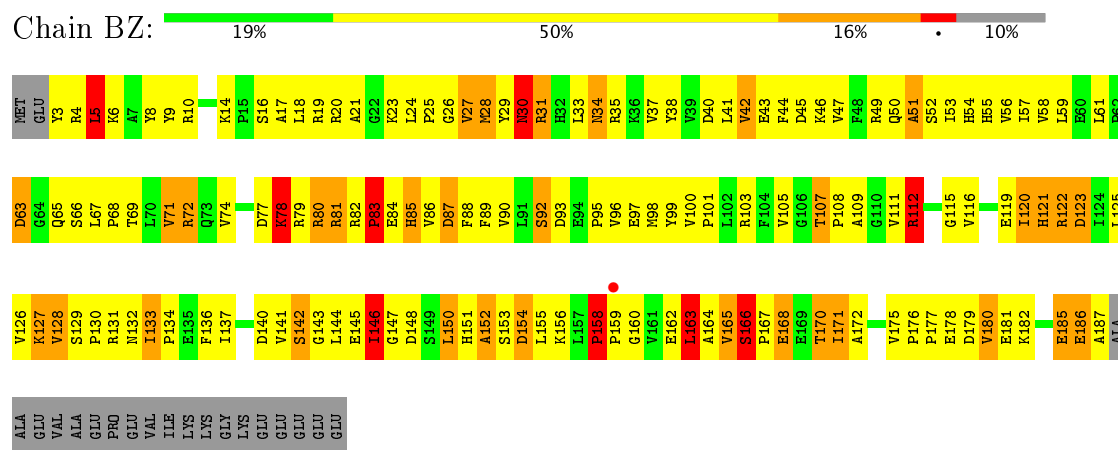
- Molecule 57: 50S RIBOSOMAL PROTEIN L24



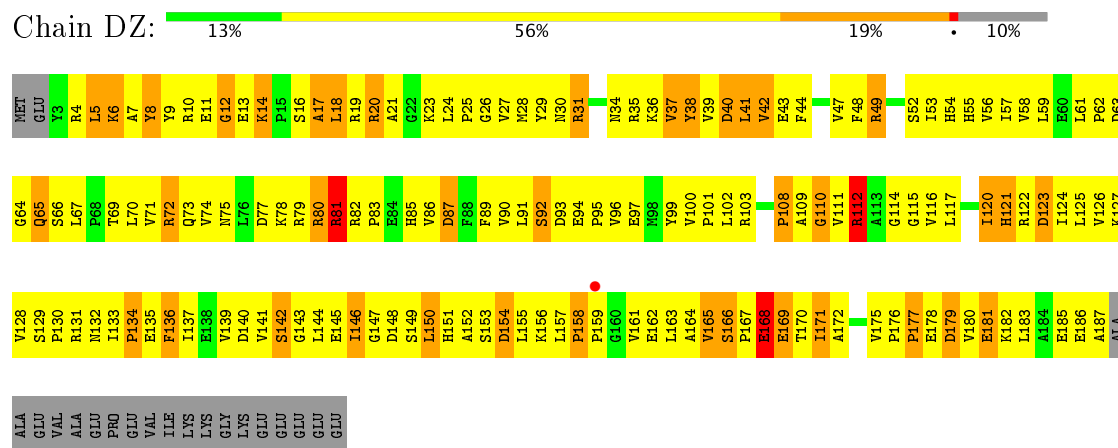
• Molecule 57: 50S RIBOSOMAL PROTEIN L24



• Molecule 58: 50S RIBOSOMAL PROTEIN L25



• Molecule 58: 50S RIBOSOMAL PROTEIN L25



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1 21 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 291.84Å 270.36Å 402.36Å<br>90.00° 91.73° 90.00°             | Depositor        |
| Resolution (Å)  | 50.00 – 3.60<br>49.57 – 3.40                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 96.0 (50.00-3.60)<br>95.0 (49.57-3.40)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.37  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.57 (at 3.40Å)   | Xtriage          |
| Refinement program  | CNS 1.2   | Depositor        |
| R, $R_{free}$   | 0.227 , 0.260<br>0.227 , 0.227                              | Depositor<br>DCC |
| $R_{free}$ test set   | 34394 reflections (5.24%)                                   | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 78.6  | Xtriage          |
| Anisotropy  | 0.084   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.27 , 34.7   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$ | Xtriage          |
| Estimated twinning fraction   | 0.048 for h,-k,-l   | Xtriage          |
| $F_o, F_c$ correlation  | 0.90  | EDS              |
| Total number of atoms   | 311552  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 86.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.36% 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: GDP, 5MU, ZN, MG, FUA

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    | 0.61         | 1/36190 (0.0%) | 0.76        | 26/56486 (0.0%) |
| 1   | CA    | 0.60         | 2/36190 (0.0%) | 0.76        | 20/56486 (0.0%) |
| 2   | AB    | 0.46         | 0/1936         | 0.70        | 0/2611          |
| 2   | CB    | 0.44         | 0/1936         | 0.70        | 0/2611          |
| 3   | AC    | 0.52         | 0/1637         | 0.69        | 0/2207          |
| 3   | CC    | 0.46         | 0/1637         | 0.69        | 0/2207          |
| 4   | AD    | 0.42         | 0/1733         | 0.66        | 0/2318          |
| 4   | CD    | 0.41         | 0/1733         | 0.66        | 0/2318          |
| 5   | AE    | 0.59         | 0/1163         | 0.72        | 0/1566          |
| 5   | CE    | 0.55         | 0/1163         | 0.71        | 0/1566          |
| 6   | AF    | 0.44         | 0/856          | 0.67        | 0/1154          |
| 6   | CF    | 0.40         | 0/856          | 0.66        | 0/1154          |
| 7   | AG    | 0.45         | 0/1276         | 0.65        | 0/1709          |
| 7   | CG    | 0.45         | 0/1276         | 0.65        | 0/1709          |
| 8   | AH    | 0.51         | 0/1136         | 0.74        | 0/1527          |
| 8   | CH    | 0.46         | 0/1136         | 0.74        | 0/1527          |
| 9   | AI    | 0.44         | 0/1027         | 0.68        | 0/1373          |
| 9   | CI    | 0.41         | 0/1027         | 0.67        | 0/1373          |
| 10  | AJ    | 0.47         | 0/808          | 0.72        | 0/1087          |
| 10  | CJ    | 0.42         | 0/808          | 0.71        | 0/1087          |
| 11  | AK    | 0.50         | 0/900          | 0.70        | 0/1213          |
| 11  | CK    | 0.47         | 0/900          | 0.70        | 0/1213          |
| 12  | AL    | 0.52         | 0/987          | 0.75        | 0/1322          |
| 12  | CL    | 0.48         | 0/987          | 0.74        | 0/1322          |
| 13  | AM    | 0.41         | 0/999          | 0.69        | 0/1338          |
| 13  | CM    | 0.39         | 0/999          | 0.69        | 0/1338          |
| 14  | AN    | 0.49         | 0/501          | 0.69        | 0/664           |
| 14  | CN    | 0.47         | 0/501          | 0.69        | 0/664           |
| 15  | AO    | 0.45         | 0/745          | 0.67        | 0/992           |
| 15  | CO    | 0.43         | 0/745          | 0.66        | 0/992           |
| 16  | AP    | 0.45         | 0/717          | 0.68        | 0/965           |
| 16  | CP    | 0.43         | 0/717          | 0.68        | 0/965           |

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5          |
| 17  | AQ    | 0.51         | 0/837          | 0.69        | 0/1119           |
| 17  | CQ    | 0.49         | 0/837          | 0.69        | 0/1119           |
| 18  | AR    | 0.47         | 0/579          | 0.72        | 0/768            |
| 18  | CR    | 0.45         | 0/579          | 0.73        | 0/768            |
| 19  | AS    | 0.46         | 0/643          | 0.68        | 1/867 (0.1%)     |
| 19  | CS    | 0.44         | 0/643          | 0.67        | 1/867 (0.1%)     |
| 20  | AT    | 0.40         | 0/765          | 0.66        | 0/1007           |
| 20  | CT    | 0.39         | 0/765          | 0.66        | 0/1007           |
| 21  | AU    | 0.52         | 0/213          | 0.65        | 0/279            |
| 21  | CU    | 0.50         | 0/213          | 0.65        | 0/279            |
| 22  | AV    | 0.57         | 0/1810         | 0.73        | 0/2821           |
| 22  | AW    | 0.41         | 0/1810         | 0.72        | 0/2821           |
| 22  | CV    | 0.54         | 0/1810         | 0.70        | 0/2821           |
| 22  | CW    | 0.38         | 0/1810         | 0.69        | 0/2821           |
| 23  | AX    | 0.82         | 0/257          | 0.86        | 0/398            |
| 23  | CX    | 0.79         | 0/257          | 0.84        | 1/398 (0.3%)     |
| 24  | AY    | 0.40         | 0/5313         | 0.69        | 0/7195           |
| 24  | CY    | 0.42         | 0/5313         | 0.69        | 1/7195 (0.0%)    |
| 25  | B0    | 0.43         | 0/671          | 0.66        | 0/892            |
| 25  | D0    | 0.42         | 0/671          | 0.67        | 0/892            |
| 26  | B1    | 0.48         | 0/739          | 0.78        | 0/983            |
| 26  | D1    | 0.45         | 0/739          | 0.69        | 0/983            |
| 27  | B2    | 0.36         | 0/600          | 0.66        | 0/793            |
| 27  | D2    | 0.37         | 0/600          | 0.62        | 0/793            |
| 28  | B3    | 0.43         | 0/473          | 0.63        | 0/636            |
| 28  | D3    | 0.43         | 0/473          | 0.64        | 0/636            |
| 29  | B4    | 0.68         | 0/461          | 0.92        | 2/623 (0.3%)     |
| 29  | D4    | 0.74         | 0/461          | 0.93        | 2/623 (0.3%)     |
| 30  | B5    | 0.43         | 0/473          | 0.75        | 0/639            |
| 30  | D5    | 0.44         | 0/473          | 0.74        | 0/639            |
| 31  | B6    | 0.64         | 0/440          | 0.96        | 1/586 (0.2%)     |
| 31  | D6    | 0.64         | 0/440          | 0.96        | 1/586 (0.2%)     |
| 32  | B7    | 0.45         | 0/427          | 0.71        | 0/563            |
| 32  | D7    | 0.45         | 0/427          | 0.71        | 0/563            |
| 33  | B8    | 0.54         | 0/516          | 0.83        | 0/681            |
| 33  | D8    | 0.54         | 0/516          | 0.83        | 0/681            |
| 34  | B9    | 0.47         | 0/310          | 0.69        | 0/407            |
| 34  | D9    | 0.46         | 0/310          | 0.70        | 0/407            |
| 35  | BA    | 0.56         | 3/69972 (0.0%) | 0.75        | 35/109237 (0.0%) |
| 35  | DA    | 0.55         | 4/69972 (0.0%) | 0.75        | 36/109237 (0.0%) |
| 36  | BB    | 0.44         | 0/2853         | 0.72        | 1/4451 (0.0%)    |
| 36  | DB    | 0.44         | 0/2853         | 0.72        | 0/4451           |
| 37  | BC    | 0.35         | 0/1774         | 0.61        | 0/2391           |



| Mol | Chain | Bond lengths |                  | Bond angles |                   |
|-----|-------|--------------|------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5           |
| 37  | DC    | 0.34         | 0/1774           | 0.61        | 0/2391            |
| 38  | BD    | 0.54         | 0/2195           | 0.83        | 0/2955            |
| 38  | DD    | 0.53         | 0/2195           | 0.82        | 0/2955            |
| 39  | BE    | 0.48         | 0/1597           | 0.74        | 0/2155            |
| 39  | DE    | 0.46         | 0/1597           | 0.74        | 0/2155            |
| 40  | BF    | 0.39         | 0/1659           | 0.66        | 0/2246            |
| 40  | DF    | 0.38         | 0/1659           | 0.66        | 0/2246            |
| 41  | BG    | 0.42         | 0/1498           | 0.78        | 1/2013 (0.0%)     |
| 41  | DG    | 0.43         | 0/1498           | 0.74        | 0/2013            |
| 42  | BH    | 0.36         | 0/1293           | 0.71        | 0/1746            |
| 42  | DH    | 0.35         | 0/1293           | 0.69        | 0/1746            |
| 44  | BK    | 0.35         | 0/1045           | 0.60        | 0/1418            |
| 44  | DK    | 0.36         | 0/1045           | 0.60        | 0/1418            |
| 46  | BN    | 0.40         | 0/1132           | 0.73        | 1/1527 (0.1%)     |
| 46  | DN    | 0.39         | 0/1132           | 0.73        | 1/1527 (0.1%)     |
| 47  | BO    | 0.49         | 0/943            | 0.72        | 0/1269            |
| 47  | DO    | 0.47         | 0/943            | 0.72        | 0/1269            |
| 48  | BP    | 0.44         | 0/1131           | 0.93        | 4/1504 (0.3%)     |
| 48  | DP    | 0.44         | 0/1131           | 0.91        | 4/1504 (0.3%)     |
| 49  | BQ    | 0.49         | 0/1143           | 0.69        | 0/1527            |
| 49  | DQ    | 0.48         | 0/1143           | 0.70        | 0/1527            |
| 50  | BR    | 0.39         | 0/974            | 0.68        | 0/1302            |
| 50  | DR    | 0.38         | 0/974            | 0.68        | 1/1302 (0.1%)     |
| 51  | BS    | 0.41         | 0/779            | 0.69        | 0/1038            |
| 51  | DS    | 0.40         | 0/779            | 0.70        | 0/1038            |
| 52  | BT    | 0.47         | 0/1156           | 0.79        | 2/1544 (0.1%)     |
| 52  | DT    | 0.49         | 0/1156           | 0.79        | 1/1544 (0.1%)     |
| 53  | BU    | 0.43         | 0/975            | 0.68        | 0/1297            |
| 53  | DU    | 0.44         | 0/975            | 0.69        | 0/1297            |
| 54  | BV    | 0.39         | 0/790            | 0.70        | 0/1057            |
| 54  | DV    | 0.39         | 0/790            | 0.70        | 0/1057            |
| 55  | BW    | 0.37         | 0/907            | 0.65        | 0/1216            |
| 55  | DW    | 0.39         | 0/907            | 0.65        | 0/1216            |
| 56  | BX    | 0.42         | 0/740            | 0.66        | 0/995             |
| 56  | DX    | 0.42         | 0/740            | 0.66        | 0/995             |
| 57  | BY    | 0.41         | 0/824            | 0.67        | 0/1100            |
| 57  | DY    | 0.42         | 0/824            | 0.68        | 0/1100            |
| 58  | BZ    | 0.48         | 0/1500           | 0.74        | 0/2037            |
| 58  | DZ    | 0.46         | 0/1500           | 0.73        | 0/2037            |
| All | All   | 0.53         | 10/333656 (0.0%) | 0.74        | 143/497270 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | AA    | 0                   | 48                  |
| 1   | CA    | 0                   | 43                  |
| 22  | AV    | 0                   | 3                   |
| 22  | CV    | 0                   | 1                   |
| 23  | AX    | 0                   | 2                   |
| 23  | CX    | 0                   | 1                   |
| 35  | BA    | 2                   | 69                  |
| 35  | DA    | 2                   | 58                  |
| 36  | BB    | 0                   | 1                   |
| 36  | DB    | 0                   | 1                   |
| 37  | BC    | 0                   | 1                   |
| 37  | DC    | 0                   | 1                   |
| 44  | BK    | 0                   | 1                   |
| 44  | DK    | 0                   | 1                   |
| 46  | DN    | 0                   | 1                   |
| All | All   | 4                   | 232                 |

All (10) bond length outliers are listed below:

| Mol | Chain | Res    | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|--------|-------|-------------|----------|
| 35  | BA    | 2506   | U    | N1-C2  | 7.05  | 1.44        | 1.38     |
| 35  | DA    | 2506   | U    | N1-C2  | 6.48  | 1.44        | 1.38     |
| 35  | BA    | 272(I) | U    | C1'-N1 | 5.69  | 1.57        | 1.48     |
| 1   | AA    | 1417   | G    | C6-O6  | 5.55  | 1.29        | 1.24     |
| 35  | DA    | 272(I) | U    | C1'-N1 | 5.49  | 1.56        | 1.48     |
| 35  | DA    | 1786   | A    | C5-C6  | -5.20 | 1.36        | 1.41     |
| 35  | DA    | 1671   | U    | N3-C4  | 5.12  | 1.43        | 1.38     |
| 1   | CA    | 1108   | G    | C5-C6  | 5.04  | 1.47        | 1.42     |
| 1   | CA    | 299    | G    | C6-O6  | 5.03  | 1.28        | 1.24     |
| 35  | BA    | 1828   | G    | P-OP2  | 5.02  | 1.57        | 1.49     |

All (143) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BA    | 1992 | G    | C2'-C3'-O3' | 10.77 | 133.19      | 109.50   |
| 35  | DA    | 1992 | G    | C2'-C3'-O3' | 10.61 | 132.85      | 109.50   |
| 1   | CA    | 575  | G    | C2'-C3'-O3' | 9.68  | 130.80      | 109.50   |
| 1   | AA    | 575  | G    | C2'-C3'-O3' | 9.65  | 130.72      | 109.50   |
| 35  | BA    | 945  | A    | N9-C1'-C2'  | 9.34  | 126.14      | 114.00   |
| 35  | DA    | 945  | A    | N9-C1'-C2'  | 9.33  | 126.13      | 114.00   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | DA    | 1799 | G    | C2'-C3'-O3' | 9.18  | 129.70      | 109.50   |
| 35  | BA    | 1799 | G    | C2'-C3'-O3' | 9.10  | 129.52      | 109.50   |
| 1   | CA    | 1498 | U    | C2'-C3'-O3' | 9.09  | 129.49      | 109.50   |
| 1   | AA    | 1498 | U    | C2'-C3'-O3' | 8.88  | 129.05      | 109.50   |
| 1   | AA    | 115  | G    | C2'-C3'-O3' | 8.46  | 128.11      | 109.50   |
| 35  | DA    | 1379 | A    | N9-C1'-C2'  | 8.43  | 124.96      | 114.00   |
| 1   | CA    | 115  | G    | C2'-C3'-O3' | 8.27  | 127.69      | 109.50   |
| 35  | BA    | 1379 | A    | N9-C1'-C2'  | 8.20  | 124.66      | 114.00   |
| 35  | DA    | 1786 | A    | N9-C1'-C2'  | 7.82  | 124.16      | 114.00   |
| 35  | BA    | 1786 | A    | N9-C1'-C2'  | 7.61  | 123.89      | 114.00   |
| 1   | AA    | 1502 | A    | N9-C1'-C2'  | 7.58  | 123.85      | 114.00   |
| 35  | DA    | 2799 | C    | C2'-C3'-O3' | 7.49  | 125.97      | 109.50   |
| 35  | BA    | 2799 | C    | C2'-C3'-O3' | 7.44  | 125.87      | 109.50   |
| 36  | BB    | 103  | G    | C5'-C4'-C3' | -7.43 | 104.11      | 116.00   |
| 35  | BA    | 1156 | A    | N9-C1'-C2'  | 7.15  | 123.29      | 114.00   |
| 35  | DA    | 1156 | A    | N9-C1'-C2'  | 7.11  | 123.25      | 114.00   |
| 1   | CA    | 60   | A    | C2'-C3'-O3' | 7.11  | 125.14      | 109.50   |
| 48  | BP    | 53   | GLY  | N-CA-C      | -7.06 | 95.45       | 113.10   |
| 1   | AA    | 60   | A    | C2'-C3'-O3' | 7.04  | 124.99      | 109.50   |
| 48  | DP    | 53   | GLY  | N-CA-C      | -6.98 | 95.64       | 113.10   |
| 1   | CA    | 921  | U    | C5'-C4'-C3' | -6.96 | 104.86      | 116.00   |
| 1   | AA    | 921  | U    | C5'-C4'-C3' | -6.76 | 105.18      | 116.00   |
| 48  | DP    | 52   | GLU  | N-CA-C      | 6.76  | 129.25      | 111.00   |
| 48  | BP    | 52   | GLU  | N-CA-C      | 6.72  | 129.15      | 111.00   |
| 35  | DA    | 1654 | A    | C5'-C4'-C3' | 6.65  | 126.64      | 116.00   |
| 35  | BA    | 788  | A    | N9-C1'-C2'  | 6.55  | 122.51      | 114.00   |
| 35  | BA    | 1396 | U    | N1-C1'-C2'  | 6.51  | 122.46      | 114.00   |
| 35  | BA    | 1654 | A    | C5'-C4'-C3' | 6.48  | 126.37      | 116.00   |
| 1   | AA    | 1285 | A    | C2'-C3'-O3' | 6.45  | 124.02      | 113.70   |
| 1   | CA    | 1505 | G    | O5'-P-OP1   | -6.43 | 99.91       | 105.70   |
| 35  | DA    | 1020 | A    | N9-C1'-C2'  | 6.43  | 122.36      | 114.00   |
| 1   | CA    | 792  | A    | C5'-C4'-C3' | -6.36 | 105.83      | 116.00   |
| 35  | DA    | 1396 | U    | N1-C1'-C2'  | 6.35  | 122.25      | 114.00   |
| 1   | AA    | 1457 | G    | N9-C1'-C2'  | -6.33 | 105.03      | 112.00   |
| 19  | AS    | 5    | LEU  | CA-CB-CG    | 6.33  | 129.85      | 115.30   |
| 1   | AA    | 792  | A    | C5'-C4'-C3' | -6.31 | 105.90      | 116.00   |
| 35  | BA    | 1236 | G    | N9-C1'-C2'  | 6.30  | 122.20      | 114.00   |
| 31  | D6    | 23   | THR  | N-CA-C      | 6.29  | 127.98      | 111.00   |
| 1   | AA    | 328  | C    | C2'-C3'-O3' | 6.28  | 123.75      | 113.70   |
| 35  | BA    | 49   | A    | C2'-C3'-O3' | 6.28  | 123.75      | 113.70   |
| 1   | CA    | 533  | A    | C2'-C3'-O3' | 6.27  | 123.73      | 113.70   |
| 29  | B4    | 43   | TYR  | N-CA-C      | 6.26  | 127.92      | 111.00   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 31  | B6    | 23   | THR  | N-CA-C      | 6.24  | 127.86      | 111.00   |
| 29  | D4    | 43   | TYR  | N-CA-C      | 6.23  | 127.82      | 111.00   |
| 1   | AA    | 1190 | G    | N9-C1'-C2'  | 6.21  | 122.07      | 114.00   |
| 1   | AA    | 1201 | A    | C2'-C3'-O3' | 6.20  | 123.62      | 113.70   |
| 35  | BA    | 1020 | A    | N9-C1'-C2'  | 6.17  | 122.03      | 114.00   |
| 35  | DA    | 788  | A    | N9-C1'-C2'  | 6.15  | 122.00      | 114.00   |
| 35  | BA    | 2732 | G    | N9-C1'-C2'  | 6.14  | 121.99      | 114.00   |
| 35  | DA    | 945  | A    | O4'-C1'-N9  | 6.06  | 113.05      | 108.20   |
| 35  | DA    | 1236 | G    | N9-C1'-C2'  | 6.06  | 121.87      | 114.00   |
| 48  | DP    | 58   | THR  | N-CA-C      | -6.03 | 94.73       | 111.00   |
| 1   | CA    | 428  | G    | C2'-C3'-O3' | 6.02  | 123.33      | 113.70   |
| 1   | CA    | 1502 | A    | N9-C1'-C2'  | 6.02  | 121.82      | 114.00   |
| 35  | BA    | 945  | A    | O4'-C1'-N9  | 6.00  | 113.00      | 108.20   |
| 35  | BA    | 2225 | A    | C2'-C3'-O3' | 6.00  | 123.29      | 113.70   |
| 1   | CA    | 1190 | G    | N9-C1'-C2'  | 5.99  | 121.78      | 114.00   |
| 35  | DA    | 1819 | A    | N9-C1'-C2'  | 5.99  | 121.79      | 114.00   |
| 1   | AA    | 533  | A    | C2'-C3'-O3' | 5.95  | 123.22      | 113.70   |
| 35  | DA    | 49   | A    | C2'-C3'-O3' | 5.95  | 123.22      | 113.70   |
| 1   | CA    | 1493 | A    | C2'-C3'-O3' | 5.95  | 123.22      | 113.70   |
| 1   | CA    | 204  | U    | O4'-C1'-N1  | 5.94  | 112.95      | 108.20   |
| 35  | BA    | 1493 | C    | N1-C1'-C2'  | 5.93  | 121.71      | 114.00   |
| 1   | AA    | 1109 | C    | OP2-P-O3'   | 5.93  | 118.24      | 105.20   |
| 48  | BP    | 58   | THR  | N-CA-C      | -5.93 | 95.00       | 111.00   |
| 1   | CA    | 328  | C    | C2'-C3'-O3' | 5.92  | 123.18      | 113.70   |
| 1   | AA    | 428  | G    | C2'-C3'-O3' | 5.85  | 123.05      | 113.70   |
| 19  | CS    | 5    | LEU  | CA-CB-CG    | 5.84  | 128.74      | 115.30   |
| 1   | AA    | 1398 | A    | C5'-C4'-C3' | -5.84 | 106.66      | 116.00   |
| 35  | BA    | 1819 | A    | N9-C1'-C2'  | 5.84  | 121.59      | 114.00   |
| 35  | DA    | 2732 | G    | N9-C1'-C2'  | 5.81  | 121.56      | 114.00   |
| 35  | DA    | 1493 | C    | N1-C1'-C2'  | 5.78  | 121.51      | 114.00   |
| 35  | BA    | 2172 | U    | C2'-C3'-O3' | 5.75  | 122.91      | 113.70   |
| 1   | CA    | 1285 | A    | C2'-C3'-O3' | 5.75  | 122.90      | 113.70   |
| 1   | AA    | 204  | U    | O4'-C1'-N1  | 5.72  | 112.78      | 108.20   |
| 35  | BA    | 1252 | G    | N9-C1'-C2'  | 5.71  | 121.42      | 114.00   |
| 35  | DA    | 2225 | A    | C2'-C3'-O3' | 5.71  | 122.83      | 113.70   |
| 35  | BA    | 2835 | A    | N9-C1'-C2'  | 5.70  | 121.41      | 114.00   |
| 1   | AA    | 30   | U    | N1-C1'-C2'  | 5.70  | 121.41      | 114.00   |
| 35  | BA    | 1838 | C    | C2'-C3'-O3' | 5.69  | 122.81      | 113.70   |
| 1   | CA    | 1201 | A    | C2'-C3'-O3' | 5.68  | 122.79      | 113.70   |
| 35  | BA    | 2345 | G    | C1'-O4'-C4' | -5.64 | 105.39      | 109.90   |
| 35  | BA    | 2026 | C    | C5'-C4'-C3' | -5.62 | 107.02      | 116.00   |
| 35  | BA    | 479  | A    | N9-C1'-C2'  | 5.59  | 121.27      | 114.00   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | DA    | 1237 | A    | N9-C1'-C2'  | 5.58  | 121.25      | 114.00   |
| 35  | DA    | 2481 | G    | N9-C1'-C2'  | 5.56  | 121.23      | 114.00   |
| 35  | BA    | 2481 | G    | N9-C1'-C2'  | 5.54  | 121.21      | 114.00   |
| 35  | BA    | 675  | A    | N9-C1'-C2'  | 5.54  | 121.20      | 114.00   |
| 35  | BA    | 1237 | A    | N9-C1'-C2'  | 5.54  | 121.19      | 114.00   |
| 35  | DA    | 2172 | U    | C2'-C3'-O3' | 5.52  | 122.53      | 113.70   |
| 1   | CA    | 366  | C    | C2'-C3'-O3' | 5.48  | 122.47      | 113.70   |
| 35  | DA    | 1252 | G    | N9-C1'-C2'  | 5.46  | 121.10      | 114.00   |
| 35  | DA    | 479  | A    | N9-C1'-C2'  | 5.44  | 121.07      | 114.00   |
| 35  | DA    | 906  | G    | C5'-C4'-C3' | -5.43 | 107.31      | 116.00   |
| 35  | DA    | 2779 | U    | O4'-C1'-N1  | 5.42  | 112.53      | 108.20   |
| 1   | AA    | 366  | C    | C2'-C3'-O3' | 5.41  | 122.35      | 113.70   |
| 35  | DA    | 1838 | C    | C2'-C3'-O3' | 5.40  | 122.34      | 113.70   |
| 35  | DA    | 1904 | G    | C5'-C4'-C3' | -5.40 | 107.36      | 116.00   |
| 35  | BA    | 1959 | G    | C5'-C4'-C3' | -5.37 | 107.41      | 116.00   |
| 35  | BA    | 1948 | G    | C5'-C4'-O4' | -5.36 | 102.66      | 109.10   |
| 35  | DA    | 748  | G    | N9-C1'-C2'  | 5.36  | 120.97      | 114.00   |
| 23  | CX    | 11   | U    | N1-C1'-C2'  | 5.32  | 120.92      | 114.00   |
| 35  | DA    | 2835 | A    | N9-C1'-C2'  | 5.31  | 120.90      | 114.00   |
| 35  | BA    | 1818 | U    | C5'-C4'-C3' | -5.27 | 107.56      | 116.00   |
| 1   | CA    | 30   | U    | N1-C1'-C2'  | 5.26  | 120.84      | 114.00   |
| 35  | DA    | 2026 | C    | C5'-C4'-C3' | -5.25 | 107.60      | 116.00   |
| 1   | AA    | 481  | G    | C5'-C4'-C3' | -5.23 | 107.63      | 116.00   |
| 35  | DA    | 675  | A    | N9-C1'-C2'  | 5.22  | 120.79      | 114.00   |
| 46  | BN    | 3    | THR  | N-CA-C      | -5.22 | 96.92       | 111.00   |
| 52  | BT    | 29   | ARG  | N-CA-C      | 5.22  | 125.08      | 111.00   |
| 29  | D4    | 53   | GLU  | N-CA-C      | 5.21  | 125.06      | 111.00   |
| 35  | DA    | 2345 | G    | C1'-O4'-C4' | -5.18 | 105.75      | 109.90   |
| 35  | BA    | 2126 | A    | N9-C1'-C2'  | 5.18  | 120.73      | 114.00   |
| 24  | CY    | 34   | TYR  | N-CA-C      | -5.18 | 97.02       | 111.00   |
| 1   | AA    | 812  | C    | OP2-P-O3'   | 5.17  | 116.59      | 105.20   |
| 1   | AA    | 1049 | U    | N1-C1'-C2'  | 5.15  | 120.70      | 114.00   |
| 35  | BA    | 2779 | U    | O4'-C1'-N1  | 5.15  | 112.32      | 108.20   |
| 1   | AA    | 1065 | U    | N1-C1'-C2'  | 5.15  | 120.69      | 114.00   |
| 35  | DA    | 2035 | G    | N9-C1'-C2'  | 5.15  | 120.69      | 114.00   |
| 46  | DN    | 3    | THR  | N-CA-C      | -5.15 | 97.10       | 111.00   |
| 1   | CA    | 1049 | U    | N1-C1'-C2'  | 5.14  | 120.68      | 114.00   |
| 52  | DT    | 29   | ARG  | N-CA-C      | 5.13  | 124.86      | 111.00   |
| 48  | DP    | 41   | ARG  | N-CA-C      | -5.12 | 97.17       | 111.00   |
| 35  | BA    | 1459 | G    | N9-C1'-C2'  | 5.10  | 120.63      | 114.00   |
| 41  | BG    | 139  | LEU  | CA-CB-CG    | 5.09  | 127.01      | 115.30   |
| 1   | AA    | 1498 | U    | OP2-P-O3'   | 5.09  | 116.39      | 105.20   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 29  | B4    | 53   | GLU  | N-CA-C      | 5.07  | 124.70      | 111.00   |
| 35  | DA    | 1948 | G    | C5'-C4'-O4' | -5.06 | 103.03      | 109.10   |
| 48  | BP    | 41   | ARG  | N-CA-C      | -5.05 | 97.36       | 111.00   |
| 35  | DA    | 1654 | A    | N9-C1'-C2'  | -5.03 | 106.47      | 112.00   |
| 1   | AA    | 754  | C    | N1-C1'-C2'  | 5.03  | 120.53      | 114.00   |
| 1   | AA    | 1456 | G    | N9-C1'-C2'  | 5.03  | 120.53      | 114.00   |
| 1   | CA    | 754  | C    | N1-C1'-C2'  | 5.02  | 120.53      | 114.00   |
| 50  | DR    | 4    | LEU  | CA-CB-CG    | 5.02  | 126.85      | 115.30   |
| 35  | DA    | 1351 | C    | C5'-C4'-C3' | -5.01 | 107.98      | 116.00   |
| 52  | BT    | 80   | SER  | N-CA-C      | 5.01  | 124.53      | 111.00   |
| 35  | BA    | 848  | G    | C5'-C4'-C3' | -5.00 | 107.99      | 116.00   |

All (4) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 35  | BA    | 1799 | G    | C3'  |
| 35  | BA    | 1992 | G    | C3'  |
| 35  | DA    | 1799 | G    | C3'  |
| 35  | DA    | 1992 | G    | C3'  |

All (232) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | AA    | 1053 | G    | Sidechain |
| 1   | AA    | 1055 | A    | Sidechain |
| 1   | AA    | 1077 | G    | Sidechain |
| 1   | AA    | 108  | G    | Sidechain |
| 1   | AA    | 1109 | C    | Sidechain |
| 1   | AA    | 112  | G    | Sidechain |
| 1   | AA    | 1184 | G    | Sidechain |
| 1   | AA    | 1190 | G    | Sidechain |
| 1   | AA    | 1219 | U    | Sidechain |
| 1   | AA    | 1226 | C    | Sidechain |
| 1   | AA    | 1331 | G    | Sidechain |
| 1   | AA    | 1355 | G    | Sidechain |
| 1   | AA    | 1370 | G    | Sidechain |
| 1   | AA    | 1391 | U    | Sidechain |
| 1   | AA    | 1401 | G    | Sidechain |
| 1   | AA    | 1402 | C    | Sidechain |
| 1   | AA    | 1403 | C    | Sidechain |
| 1   | AA    | 1414 | U    | Sidechain |
| 1   | AA    | 1485 | U    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res     | Type | Group     |
|-----|-------|---------|------|-----------|
| 1   | AA    | 1498    | U    | Sidechain |
| 1   | AA    | 1502    | A    | Sidechain |
| 1   | AA    | 1512    | U    | Sidechain |
| 1   | AA    | 1519    | A    | Sidechain |
| 1   | AA    | 30      | U    | Sidechain |
| 1   | AA    | 309     | G    | Sidechain |
| 1   | AA    | 361     | G    | Sidechain |
| 1   | AA    | 387     | U    | Sidechain |
| 1   | AA    | 39      | G    | Sidechain |
| 1   | AA    | 436     | C    | Sidechain |
| 1   | AA    | 5       | U    | Sidechain |
| 1   | AA    | 573     | A    | Sidechain |
| 1   | AA    | 582     | U    | Sidechain |
| 1   | AA    | 598     | U    | Sidechain |
| 1   | AA    | 672     | U    | Sidechain |
| 1   | AA    | 691     | G    | Sidechain |
| 1   | AA    | 724     | G    | Sidechain |
| 1   | AA    | 741     | G    | Sidechain |
| 1   | AA    | 748     | C    | Sidechain |
| 1   | AA    | 760     | G    | Sidechain |
| 1   | AA    | 781     | A    | Sidechain |
| 1   | AA    | 835     | U    | Sidechain |
| 1   | AA    | 887     | G    | Sidechain |
| 1   | AA    | 898     | G    | Sidechain |
| 1   | AA    | 963     | G    | Sidechain |
| 1   | AA    | 969     | A    | Sidechain |
| 1   | AA    | 971     | G    | Sidechain |
| 1   | AA    | 981     | U    | Sidechain |
| 1   | AA    | 991     | U    | Sidechain |
| 22  | AV    | 29      | G    | Sidechain |
| 22  | AV    | 4       | G    | Sidechain |
| 22  | AV    | 8       | U    | Sidechain |
| 23  | AX    | 12      | A    | Sidechain |
| 23  | AX    | 17      | U    | Sidechain |
| 35  | BA    | 1142(A) | A    | Sidechain |
| 35  | BA    | 1156    | A    | Sidechain |
| 35  | BA    | 1215    | G    | Sidechain |
| 35  | BA    | 1236    | G    | Sidechain |
| 35  | BA    | 1238    | G    | Sidechain |
| 35  | BA    | 1253    | A    | Sidechain |
| 35  | BA    | 1302    | A    | Sidechain |
| 35  | BA    | 1379    | A    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 35  | BA    | 1496 | A    | Sidechain |
| 35  | BA    | 1614 | A    | Sidechain |
| 35  | BA    | 1623 | G    | Sidechain |
| 35  | BA    | 1633 | G    | Sidechain |
| 35  | BA    | 1645 | G    | Sidechain |
| 35  | BA    | 1772 | G    | Sidechain |
| 35  | BA    | 1776 | G    | Sidechain |
| 35  | BA    | 1781 | C    | Sidechain |
| 35  | BA    | 1822 | G    | Sidechain |
| 35  | BA    | 1827 | C    | Sidechain |
| 35  | BA    | 1919 | A    | Sidechain |
| 35  | BA    | 1920 | C    | Sidechain |
| 35  | BA    | 1926 | U    | Sidechain |
| 35  | BA    | 1929 | G    | Sidechain |
| 35  | BA    | 1952 | A    | Sidechain |
| 35  | BA    | 1992 | G    | Sidechain |
| 35  | BA    | 200  | U    | Sidechain |
| 35  | BA    | 2009 | G    | Sidechain |
| 35  | BA    | 2010 | G    | Sidechain |
| 35  | BA    | 2031 | A    | Sidechain |
| 35  | BA    | 2051 | A    | Sidechain |
| 35  | BA    | 2052 | G    | Sidechain |
| 35  | BA    | 2053 | G    | Sidechain |
| 35  | BA    | 2059 | A    | Sidechain |
| 35  | BA    | 2079 | U    | Sidechain |
| 35  | BA    | 2126 | A    | Sidechain |
| 35  | BA    | 2250 | G    | Sidechain |
| 35  | BA    | 2266 | A    | Sidechain |
| 35  | BA    | 2296 | U    | Sidechain |
| 35  | BA    | 2340 | G    | Sidechain |
| 35  | BA    | 2344 | U    | Sidechain |
| 35  | BA    | 2401 | U    | Sidechain |
| 35  | BA    | 2464 | C    | Sidechain |
| 35  | BA    | 248  | G    | Sidechain |
| 35  | BA    | 2481 | G    | Sidechain |
| 35  | BA    | 2494 | G    | Sidechain |
| 35  | BA    | 2504 | U    | Sidechain |
| 35  | BA    | 2506 | U    | Sidechain |
| 35  | BA    | 2508 | G    | Sidechain |
| 35  | BA    | 2518 | A    | Sidechain |
| 35  | BA    | 2564 | A    | Sidechain |
| 35  | BA    | 2569 | G    | Sidechain |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 35  | BA    | 2609 | U    | Sidechain |
| 35  | BA    | 2659 | G    | Sidechain |
| 35  | BA    | 2685 | G    | Sidechain |
| 35  | BA    | 2826 | A    | Sidechain |
| 35  | BA    | 2835 | A    | Sidechain |
| 35  | BA    | 395  | U    | Sidechain |
| 35  | BA    | 463  | G    | Sidechain |
| 35  | BA    | 528  | A    | Sidechain |
| 35  | BA    | 562  | U    | Sidechain |
| 35  | BA    | 686  | G    | Sidechain |
| 35  | BA    | 688  | U    | Sidechain |
| 35  | BA    | 742  | G    | Sidechain |
| 35  | BA    | 788  | A    | Sidechain |
| 35  | BA    | 83   | G    | Sidechain |
| 35  | BA    | 845  | G    | Sidechain |
| 35  | BA    | 895  | U    | Sidechain |
| 35  | BA    | 913  | U    | Sidechain |
| 35  | BA    | 945  | A    | Sidechain |
| 35  | BA    | 958  | U    | Sidechain |
| 36  | BB    | 21   | G    | Sidechain |
| 37  | BC    | 28   | ARG  | Sidechain |
| 44  | BK    | 6    | ALA  | Peptide   |
| 1   | CA    | 1053 | G    | Sidechain |
| 1   | CA    | 1077 | G    | Sidechain |
| 1   | CA    | 1190 | G    | Sidechain |
| 1   | CA    | 1226 | C    | Sidechain |
| 1   | CA    | 1231 | G    | Sidechain |
| 1   | CA    | 1331 | G    | Sidechain |
| 1   | CA    | 1355 | G    | Sidechain |
| 1   | CA    | 1370 | G    | Sidechain |
| 1   | CA    | 1502 | A    | Sidechain |
| 1   | CA    | 1505 | G    | Sidechain |
| 1   | CA    | 1512 | U    | Sidechain |
| 1   | CA    | 1519 | A    | Sidechain |
| 1   | CA    | 1525 | G    | Sidechain |
| 1   | CA    | 1527 | C    | Sidechain |
| 1   | CA    | 204  | U    | Sidechain |
| 1   | CA    | 223  | U    | Sidechain |
| 1   | CA    | 250  | A    | Sidechain |
| 1   | CA    | 253  | U    | Sidechain |
| 1   | CA    | 30   | U    | Sidechain |
| 1   | CA    | 309  | G    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | CA    | 361  | G    | Sidechain |
| 1   | CA    | 39   | G    | Sidechain |
| 1   | CA    | 436  | C    | Sidechain |
| 1   | CA    | 5    | U    | Sidechain |
| 1   | CA    | 548  | G    | Sidechain |
| 1   | CA    | 573  | A    | Sidechain |
| 1   | CA    | 582  | U    | Sidechain |
| 1   | CA    | 598  | U    | Sidechain |
| 1   | CA    | 641  | U    | Sidechain |
| 1   | CA    | 657  | G    | Sidechain |
| 1   | CA    | 672  | U    | Sidechain |
| 1   | CA    | 691  | G    | Sidechain |
| 1   | CA    | 724  | G    | Sidechain |
| 1   | CA    | 727  | G    | Sidechain |
| 1   | CA    | 741  | G    | Sidechain |
| 1   | CA    | 760  | G    | Sidechain |
| 1   | CA    | 781  | A    | Sidechain |
| 1   | CA    | 835  | U    | Sidechain |
| 1   | CA    | 887  | G    | Sidechain |
| 1   | CA    | 898  | G    | Sidechain |
| 1   | CA    | 931  | C    | Sidechain |
| 1   | CA    | 971  | G    | Sidechain |
| 1   | CA    | 991  | U    | Sidechain |
| 22  | CV    | 4    | G    | Sidechain |
| 23  | CX    | 11   | U    | Sidechain |
| 35  | DA    | 1156 | A    | Sidechain |
| 35  | DA    | 1236 | G    | Sidechain |
| 35  | DA    | 1238 | G    | Sidechain |
| 35  | DA    | 1302 | A    | Sidechain |
| 35  | DA    | 1379 | A    | Sidechain |
| 35  | DA    | 1614 | A    | Sidechain |
| 35  | DA    | 1623 | G    | Sidechain |
| 35  | DA    | 1645 | G    | Sidechain |
| 35  | DA    | 1772 | G    | Sidechain |
| 35  | DA    | 1776 | G    | Sidechain |
| 35  | DA    | 1781 | C    | Sidechain |
| 35  | DA    | 1822 | G    | Sidechain |
| 35  | DA    | 1907 | G    | Sidechain |
| 35  | DA    | 1919 | A    | Sidechain |
| 35  | DA    | 1920 | C    | Sidechain |
| 35  | DA    | 1926 | U    | Sidechain |
| 35  | DA    | 1952 | A    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 35  | DA    | 1992 | G    | Sidechain |
| 35  | DA    | 2009 | G    | Sidechain |
| 35  | DA    | 2010 | G    | Sidechain |
| 35  | DA    | 2031 | A    | Sidechain |
| 35  | DA    | 2051 | A    | Sidechain |
| 35  | DA    | 2052 | G    | Sidechain |
| 35  | DA    | 2053 | G    | Sidechain |
| 35  | DA    | 2059 | A    | Sidechain |
| 35  | DA    | 2061 | G    | Sidechain |
| 35  | DA    | 2079 | U    | Sidechain |
| 35  | DA    | 2126 | A    | Sidechain |
| 35  | DA    | 2250 | G    | Sidechain |
| 35  | DA    | 2266 | A    | Sidechain |
| 35  | DA    | 2340 | G    | Sidechain |
| 35  | DA    | 2344 | U    | Sidechain |
| 35  | DA    | 2401 | U    | Sidechain |
| 35  | DA    | 2464 | C    | Sidechain |
| 35  | DA    | 248  | G    | Sidechain |
| 35  | DA    | 2481 | G    | Sidechain |
| 35  | DA    | 2494 | G    | Sidechain |
| 35  | DA    | 2506 | U    | Sidechain |
| 35  | DA    | 2508 | G    | Sidechain |
| 35  | DA    | 2518 | A    | Sidechain |
| 35  | DA    | 2659 | G    | Sidechain |
| 35  | DA    | 2685 | G    | Sidechain |
| 35  | DA    | 2732 | G    | Sidechain |
| 35  | DA    | 2835 | A    | Sidechain |
| 35  | DA    | 395  | U    | Sidechain |
| 35  | DA    | 463  | G    | Sidechain |
| 35  | DA    | 528  | A    | Sidechain |
| 35  | DA    | 686  | G    | Sidechain |
| 35  | DA    | 688  | U    | Sidechain |
| 35  | DA    | 690  | G    | Sidechain |
| 35  | DA    | 742  | G    | Sidechain |
| 35  | DA    | 788  | A    | Sidechain |
| 35  | DA    | 83   | G    | Sidechain |
| 35  | DA    | 845  | G    | Sidechain |
| 35  | DA    | 895  | U    | Sidechain |
| 35  | DA    | 913  | U    | Sidechain |
| 35  | DA    | 945  | A    | Sidechain |
| 35  | DA    | 958  | U    | Sidechain |
| 36  | DB    | 21   | G    | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 37  | DC    | 28  | ARG  | Sidechain |
| 44  | DK    | 5   | VAL  | Peptide   |
| 46  | DN    | 72  | TYR  | 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    | 32329 | 0        | 16318    | 1236    | 0            |
| 1   | CA    | 32329 | 0        | 16318    | 1267    | 0            |
| 2   | AB    | 1901  | 0        | 1951     | 243     | 0            |
| 2   | CB    | 1901  | 0        | 1951     | 241     | 2            |
| 3   | AC    | 1613  | 0        | 1677     | 211     | 0            |
| 3   | CC    | 1613  | 0        | 1677     | 216     | 0            |
| 4   | AD    | 1703  | 0        | 1763     | 187     | 0            |
| 4   | CD    | 1703  | 0        | 1763     | 191     | 0            |
| 5   | AE    | 1147  | 0        | 1207     | 128     | 0            |
| 5   | CE    | 1147  | 0        | 1207     | 134     | 0            |
| 6   | AF    | 843   | 0        | 857      | 77      | 0            |
| 6   | CF    | 843   | 0        | 857      | 79      | 0            |
| 7   | AG    | 1257  | 0        | 1296     | 100     | 0            |
| 7   | CG    | 1257  | 0        | 1296     | 95      | 0            |
| 8   | AH    | 1116  | 0        | 1177     | 86      | 0            |
| 8   | CH    | 1116  | 0        | 1177     | 88      | 0            |
| 9   | AI    | 1010  | 0        | 1035     | 135     | 0            |
| 9   | CI    | 1010  | 0        | 1035     | 132     | 0            |
| 10  | AJ    | 795   | 0        | 840      | 180     | 0            |
| 10  | CJ    | 795   | 0        | 840      | 176     | 0            |
| 11  | AK    | 885   | 0        | 904      | 77      | 0            |
| 11  | CK    | 885   | 0        | 904      | 75      | 0            |
| 12  | AL    | 971   | 0        | 1057     | 131     | 0            |
| 12  | CL    | 971   | 0        | 1057     | 129     | 0            |
| 13  | AM    | 988   | 0        | 1059     | 146     | 0            |
| 13  | CM    | 988   | 0        | 1059     | 144     | 0            |
| 14  | AN    | 492   | 0        | 530      | 68      | 0            |
| 14  | CN    | 492   | 0        | 530      | 65      | 0            |
| 15  | AO    | 734   | 0        | 771      | 66      | 0            |
| 15  | CO    | 734   | 0        | 771      | 62      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 16  | AP    | 701   | 0        | 720      | 78      | 0            |
| 16  | CP    | 701   | 0        | 720      | 78      | 0            |
| 17  | AQ    | 824   | 0        | 891      | 60      | 0            |
| 17  | CQ    | 824   | 0        | 891      | 57      | 0            |
| 18  | AR    | 574   | 0        | 644      | 71      | 0            |
| 18  | CR    | 574   | 0        | 644      | 72      | 0            |
| 19  | AS    | 630   | 0        | 652      | 119     | 0            |
| 19  | CS    | 630   | 0        | 652      | 122     | 0            |
| 20  | AT    | 763   | 0        | 861      | 96      | 0            |
| 20  | CT    | 763   | 0        | 861      | 93      | 0            |
| 21  | AU    | 209   | 0        | 221      | 19      | 0            |
| 21  | CU    | 209   | 0        | 221      | 21      | 0            |
| 22  | AV    | 1640  | 0        | 836      | 72      | 0            |
| 22  | AW    | 1640  | 0        | 836      | 82      | 0            |
| 22  | CV    | 1640  | 0        | 836      | 49      | 0            |
| 22  | CW    | 1640  | 0        | 836      | 71      | 0            |
| 23  | AX    | 230   | 0        | 119      | 26      | 0            |
| 23  | CX    | 230   | 0        | 119      | 21      | 0            |
| 24  | AY    | 5215  | 0        | 5287     | 798     | 0            |
| 24  | CY    | 5215  | 0        | 5287     | 767     | 0            |
| 25  | B0    | 662   | 0        | 688      | 86      | 0            |
| 25  | D0    | 662   | 0        | 688      | 87      | 0            |
| 26  | B1    | 732   | 0        | 808      | 131     | 0            |
| 26  | D1    | 732   | 0        | 808      | 126     | 0            |
| 27  | B2    | 598   | 0        | 653      | 106     | 0            |
| 27  | D2    | 598   | 0        | 653      | 108     | 0            |
| 28  | B3    | 468   | 0        | 523      | 60      | 0            |
| 28  | D3    | 468   | 0        | 523      | 55      | 0            |
| 29  | B4    | 451   | 0        | 448      | 99      | 0            |
| 29  | D4    | 451   | 0        | 449      | 100     | 0            |
| 30  | B5    | 459   | 0        | 480      | 108     | 0            |
| 30  | D5    | 459   | 0        | 480      | 110     | 0            |
| 31  | B6    | 433   | 0        | 461      | 176     | 0            |
| 31  | D6    | 433   | 0        | 461      | 177     | 0            |
| 32  | B7    | 419   | 0        | 467      | 38      | 0            |
| 32  | D7    | 419   | 0        | 467      | 40      | 0            |
| 33  | B8    | 508   | 0        | 576      | 107     | 0            |
| 33  | D8    | 508   | 0        | 576      | 108     | 0            |
| 34  | B9    | 307   | 0        | 335      | 39      | 0            |
| 34  | D9    | 307   | 0        | 335      | 39      | 0            |
| 35  | BA    | 62474 | 0        | 31497    | 2701    | 0            |
| 35  | DA    | 62474 | 0        | 31497    | 2744    | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 36  | BB    | 2551  | 0        | 1295     | 127     | 0            |
| 36  | DB    | 2551  | 0        | 1295     | 135     | 0            |
| 37  | BC    | 1742  | 0        | 1798     | 169     | 0            |
| 37  | DC    | 1742  | 0        | 1798     | 168     | 2            |
| 38  | BD    | 2145  | 0        | 2234     | 302     | 0            |
| 38  | DD    | 2145  | 0        | 2234     | 306     | 0            |
| 39  | BE    | 1564  | 0        | 1629     | 280     | 0            |
| 39  | DE    | 1564  | 0        | 1629     | 282     | 0            |
| 40  | BF    | 1624  | 0        | 1677     | 261     | 0            |
| 40  | DF    | 1624  | 0        | 1677     | 269     | 0            |
| 41  | BG    | 1474  | 0        | 1534     | 288     | 0            |
| 41  | DG    | 1474  | 0        | 1534     | 272     | 0            |
| 42  | BH    | 1269  | 0        | 1337     | 231     | 0            |
| 42  | DH    | 1269  | 0        | 1337     | 216     | 0            |
| 43  | BJ    | 851   | 0        | 191      | 28      | 0            |
| 43  | DJ    | 851   | 0        | 195      | 44      | 0            |
| 44  | BK    | 1026  | 0        | 1066     | 151     | 0            |
| 44  | DK    | 1026  | 0        | 1066     | 146     | 0            |
| 45  | BL    | 506   | 0        | 111      | 14      | 0            |
| 45  | BM    | 151   | 0        | 33       | 4       | 0            |
| 45  | Bl    | 151   | 0        | 32       | 0       | 0            |
| 45  | Bm    | 146   | 0        | 32       | 0       | 0            |
| 45  | DL    | 506   | 0        | 115      | 17      | 0            |
| 45  | DM    | 151   | 0        | 32       | 1       | 0            |
| 45  | DI    | 151   | 0        | 32       | 0       | 0            |
| 45  | Dm    | 146   | 0        | 31       | 0       | 0            |
| 46  | BN    | 1105  | 0        | 1180     | 196     | 0            |
| 46  | DN    | 1105  | 0        | 1180     | 196     | 0            |
| 47  | BO    | 933   | 0        | 996      | 106     | 0            |
| 47  | DO    | 933   | 0        | 996      | 106     | 0            |
| 48  | BP    | 1114  | 0        | 1187     | 303     | 0            |
| 48  | DP    | 1114  | 0        | 1187     | 304     | 0            |
| 49  | BQ    | 1122  | 0        | 1179     | 148     | 0            |
| 49  | DQ    | 1122  | 0        | 1179     | 150     | 0            |
| 50  | BR    | 960   | 0        | 1021     | 163     | 0            |
| 50  | DR    | 960   | 0        | 1021     | 160     | 0            |
| 51  | BS    | 771   | 0        | 832      | 173     | 0            |
| 51  | DS    | 771   | 0        | 832      | 161     | 0            |
| 52  | BT    | 1142  | 0        | 1202     | 248     | 0            |
| 52  | DT    | 1142  | 0        | 1202     | 244     | 0            |
| 53  | BU    | 958   | 0        | 1015     | 171     | 0            |
| 53  | DU    | 958   | 0        | 1015     | 174     | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 54  | BV    | 779    | 0        | 852      | 140     | 0            |
| 54  | DV    | 779    | 0        | 852      | 145     | 0            |
| 55  | BW    | 896    | 0        | 953      | 97      | 0            |
| 55  | DW    | 896    | 0        | 953      | 91      | 0            |
| 56  | BX    | 726    | 0        | 778      | 78      | 0            |
| 56  | DX    | 726    | 0        | 778      | 85      | 0            |
| 57  | BY    | 811    | 0        | 901      | 171     | 0            |
| 57  | DY    | 811    | 0        | 901      | 174     | 0            |
| 58  | BZ    | 1468   | 0        | 1492     | 238     | 0            |
| 58  | DZ    | 1468   | 0        | 1492     | 275     | 0            |
| 59  | AD    | 1      | 0        | 0        | 0       | 0            |
| 59  | AN    | 1      | 0        | 0        | 1       | 0            |
| 59  | B4    | 1      | 0        | 0        | 0       | 0            |
| 59  | B9    | 1      | 0        | 0        | 0       | 0            |
| 59  | CD    | 1      | 0        | 0        | 0       | 0            |
| 59  | CN    | 1      | 0        | 0        | 0       | 0            |
| 59  | D4    | 1      | 0        | 0        | 0       | 0            |
| 59  | D9    | 1      | 0        | 0        | 0       | 0            |
| 60  | AY    | 1      | 0        | 0        | 0       | 0            |
| 60  | CY    | 1      | 0        | 0        | 0       | 0            |
| 61  | AY    | 37     | 0        | 47       | 13      | 0            |
| 61  | CY    | 37     | 0        | 47       | 22      | 0            |
| 62  | AY    | 28     | 0        | 12       | 8       | 0            |
| 62  | CY    | 28     | 0        | 12       | 8       | 0            |
| All | All   | 311552 | 0        | 214129   | 22488   | 2            |

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 (22488) 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) |
|-------------------|--------------------|--------------------------|-------------------|
| 42:DH:157:TYR:CE1 | 42:DH:171:LEU:HD22 | 1.61                     | 1.35              |
| 42:BH:157:TYR:CE1 | 42:BH:171:LEU:HD22 | 1.62                     | 1.32              |
| 42:DH:157:TYR:HE1 | 42:DH:171:LEU:CD2  | 1.50                     | 1.24              |
| 42:BH:157:TYR:HE1 | 42:BH:171:LEU:CD2  | 1.50                     | 1.24              |
| 40:DF:3:GLU:HA    | 40:DF:24:LEU:HG    | 1.24                     | 1.20              |
| 42:BH:98:LEU:HB2  | 42:BH:125:VAL:HG21 | 1.23                     | 1.19              |
| 24:AY:662:LYS:NZ  | 42:BH:175:LYS:HE3  | 1.58                     | 1.19              |
| 41:BG:68:PRO:HA   | 41:BG:92:VAL:HG12  | 1.25                     | 1.19              |
| 10:AJ:6:ILE:HD11  | 10:AJ:72:VAL:HB    | 1.23                     | 1.19              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:BE:131:ALA:HB3  | 39:BE:134:ILE:HD11 | 1.24                     | 1.18              |
| 35:DA:2012:G:H4'   | 55:DW:96:ILE:HD11  | 1.25                     | 1.17              |
| 37:BC:118:PRO:HA   | 37:BC:121:MET:CG   | 1.73                     | 1.17              |
| 56:BX:12:VAL:HB    | 56:BX:17:ALA:HB1   | 1.20                     | 1.17              |
| 42:DH:98:LEU:HB2   | 42:DH:125:VAL:HG21 | 1.21                     | 1.16              |
| 35:BA:2473:U:H3'   | 35:BA:2474:C:H5''  | 1.22                     | 1.16              |
| 1:CA:509:A:H5'     | 1:CA:510:A:OP2     | 1.45                     | 1.16              |
| 1:CA:979:C:H3'     | 1:CA:980:C:H5''    | 1.18                     | 1.15              |
| 35:BA:1378:A:O2'   | 35:BA:1379:A:H5''  | 1.45                     | 1.15              |
| 1:CA:1489:G:H2'    | 1:CA:1490:C:H5''   | 1.26                     | 1.15              |
| 24:CY:670:VAL:HG23 | 24:CY:671:MET:H    | 1.07                     | 1.15              |
| 1:AA:509:A:H5'     | 1:AA:510:A:OP2     | 1.43                     | 1.15              |
| 35:BA:2012:G:H4'   | 55:BW:96:ILE:HD11  | 1.24                     | 1.14              |
| 61:CY:702:FUA:H5   | 61:CY:702:FUA:H202 | 1.29                     | 1.14              |
| 35:DA:1043:C:H2'   | 35:DA:1044:G:H5''  | 1.27                     | 1.14              |
| 37:BC:118:PRO:HA   | 37:BC:121:MET:HG2  | 1.29                     | 1.14              |
| 23:AX:13:A:H3'     | 23:AX:14:A:H5''    | 1.30                     | 1.14              |
| 35:DA:2645:G:H3'   | 35:DA:2646:C:H5'   | 1.30                     | 1.13              |
| 35:BA:612:C:H2'    | 35:BA:613:G:H5''   | 1.22                     | 1.13              |
| 39:DE:131:ALA:HB3  | 39:DE:134:ILE:HD11 | 1.23                     | 1.12              |
| 10:CJ:6:ILE:HD11   | 10:CJ:72:VAL:HB    | 1.23                     | 1.12              |
| 35:DA:2473:U:H3'   | 35:DA:2474:C:H5''  | 1.21                     | 1.12              |
| 56:BX:12:VAL:HG23  | 56:BX:13:LEU:H     | 1.01                     | 1.12              |
| 22:AV:17:C:H5''    | 22:AV:17(A):U:H6   | 1.08                     | 1.12              |
| 24:AY:85:PRO:HA    | 24:AY:94:VAL:HG22  | 1.29                     | 1.12              |
| 41:BG:112:PRO:O    | 41:BG:113:ARG:HA   | 1.49                     | 1.12              |
| 9:CI:4:TYR:HB2     | 9:CI:19:LEU:HB2    | 1.29                     | 1.12              |
| 35:BA:903:C:H2'    | 35:BA:904:C:H5''   | 1.29                     | 1.12              |
| 23:CX:13:A:H3'     | 23:CX:14:A:C5'     | 1.80                     | 1.12              |
| 35:BA:2645:G:H3'   | 35:BA:2646:C:H5'   | 1.31                     | 1.12              |
| 40:BF:3:GLU:HA     | 40:BF:24:LEU:HG    | 1.26                     | 1.12              |
| 35:DA:903:C:H2'    | 35:DA:904:C:H5''   | 1.30                     | 1.12              |
| 35:DA:1378:A:O2'   | 35:DA:1379:A:H5''  | 1.48                     | 1.11              |
| 35:DA:996:A:H4'    | 53:DU:92:ARG:HE    | 1.02                     | 1.11              |
| 35:DA:211:A:H2'    | 35:DA:212:G:H5''   | 1.32                     | 1.11              |
| 24:AY:281:PRO:HB2  | 24:AY:286:ILE:HD11 | 1.33                     | 1.11              |
| 40:BF:53:THR:HG22  | 40:BF:56:GLU:HG3   | 1.27                     | 1.11              |
| 16:AP:20:VAL:HG21  | 16:AP:32:TYR:HB2   | 1.33                     | 1.11              |
| 50:BR:99:LYS:HD3   | 50:BR:99:LYS:H     | 1.10                     | 1.11              |
| 1:CA:656:C:H4'     | 15:CO:62:GLN:HE22  | 1.14                     | 1.11              |
| 41:BG:77:ILE:HG22  | 41:BG:80:PHE:H     | 0.96                     | 1.10              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 35:DA:2476:A:H2'    | 35:DA:2477:C:H5''  | 1.34                     | 1.10              |
| 22:AW:14:A:H2'      | 22:AW:15:G:H5''    | 1.32                     | 1.10              |
| 35:BA:996:A:H4'     | 53:BU:92:ARG:HE    | 1.03                     | 1.10              |
| 46:BN:9:VAL:HG11    | 46:BN:39:ARG:HH22  | 1.09                     | 1.10              |
| 35:DA:612:C:H2'     | 35:DA:613:G:H5''   | 1.21                     | 1.10              |
| 9:AI:4:TYR:HB2      | 9:AI:19:LEU:HB2    | 1.30                     | 1.09              |
| 35:BA:1747(A):G:H2' | 35:BA:1748:G:H5''  | 1.29                     | 1.09              |
| 38:DD:263:ARG:HB2   | 38:DD:263:ARG:HH11 | 0.96                     | 1.09              |
| 35:BA:1043:C:H2'    | 35:BA:1044:G:H5''  | 1.27                     | 1.09              |
| 40:DF:53:THR:HG22   | 40:DF:56:GLU:HG3   | 1.30                     | 1.09              |
| 61:AY:702:FUA:H202  | 61:AY:702:FUA:H5   | 1.29                     | 1.09              |
| 1:CA:793:U:H3'      | 1:CA:794:A:H5''    | 1.35                     | 1.09              |
| 35:BA:2476:A:H2'    | 35:BA:2477:C:H5''  | 1.33                     | 1.09              |
| 35:DA:1747(A):G:H2' | 35:DA:1748:G:H5''  | 1.32                     | 1.09              |
| 42:DH:157:TYR:CE1   | 42:DH:171:LEU:CD2  | 2.30                     | 1.09              |
| 35:BA:2133:G:H2'    | 35:BA:2157:G:H22   | 1.18                     | 1.09              |
| 35:DA:925:C:H2'     | 35:DA:926:A:H5''   | 1.34                     | 1.09              |
| 38:DD:35:LYS:HZ3    | 38:DD:36:PRO:HD3   | 1.14                     | 1.09              |
| 40:DF:53:THR:HG23   | 40:DF:55:GLY:H     | 1.14                     | 1.08              |
| 1:AA:979:C:H3'      | 1:AA:980:C:H5''    | 1.18                     | 1.08              |
| 35:BA:1845:G:H2'    | 35:BA:1846:G:H5''  | 1.33                     | 1.08              |
| 56:DX:12:VAL:HG23   | 56:DX:13:LEU:H     | 1.00                     | 1.08              |
| 24:AY:490:PRO:HG3   | 24:AY:516:PRO:HD2  | 1.35                     | 1.08              |
| 25:D0:11:ARG:HB2    | 25:D0:11:ARG:HH11  | 1.16                     | 1.08              |
| 35:DA:2133:G:H2'    | 35:DA:2157:G:H22   | 1.18                     | 1.08              |
| 31:B6:5:VAL:HG23    | 35:BA:2283:C:H5'   | 1.33                     | 1.08              |
| 40:BF:154:VAL:HG22  | 40:BF:191:ARG:HB3  | 1.33                     | 1.08              |
| 46:DN:9:VAL:HG11    | 46:DN:39:ARG:HH22  | 1.10                     | 1.08              |
| 22:AV:17:C:H5''     | 22:AV:17(A):U:C6   | 1.89                     | 1.08              |
| 40:BF:53:THR:HG23   | 40:BF:55:GLY:H     | 1.14                     | 1.08              |
| 58:DZ:69:THR:HG22   | 58:DZ:90:VAL:HA    | 1.28                     | 1.08              |
| 1:CA:1318:A:H1'     | 19:CS:37:ARG:HH21  | 1.15                     | 1.08              |
| 38:BD:263:ARG:HB2   | 38:BD:263:ARG:HH11 | 0.93                     | 1.07              |
| 41:BG:63:ILE:HA     | 41:BG:143:GLU:HG3  | 1.36                     | 1.07              |
| 40:DF:167:ALA:HB1   | 40:DF:173:VAL:HG11 | 1.36                     | 1.07              |
| 24:AY:157:LEU:H     | 24:AY:157:LEU:HD23 | 1.12                     | 1.07              |
| 38:BD:35:LYS:HZ3    | 38:BD:36:PRO:HD3   | 1.17                     | 1.07              |
| 50:DR:99:LYS:HD3    | 50:DR:99:LYS:H     | 1.10                     | 1.07              |
| 10:AJ:75:ILE:HG13   | 10:AJ:76:ASN:H     | 1.19                     | 1.07              |
| 16:CP:20:VAL:HG21   | 16:CP:32:TYR:HB2   | 1.32                     | 1.07              |
| 19:AS:50:ALA:HB1    | 19:AS:57:HIS:HB3   | 1.34                     | 1.07              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:AA:656:C:H4'      | 15:AO:62:GLN:HE22  | 1.18                     | 1.07              |
| 58:DZ:10:ARG:HD2    | 58:DZ:36:LYS:HE2   | 1.35                     | 1.07              |
| 56:DX:12:VAL:HB     | 56:DX:17:ALA:HB1   | 1.17                     | 1.07              |
| 35:BA:272(I):U:O4   | 35:BA:363(A):A:N1  | 1.87                     | 1.07              |
| 38:BD:263:ARG:NH1   | 38:BD:263:ARG:HB2  | 1.68                     | 1.06              |
| 1:AA:1003:G:H2'     | 1:AA:1004:A:H4'    | 1.37                     | 1.06              |
| 35:BA:925:C:H2'     | 35:BA:926:A:H5''   | 1.35                     | 1.06              |
| 35:BA:965:C:H5'     | 35:BA:2273:A:H1'   | 1.38                     | 1.06              |
| 2:CB:185:ILE:HG22   | 2:CB:199:TYR:HB2   | 1.31                     | 1.06              |
| 35:DA:272(I):U:O4   | 35:DA:363(A):A:N1  | 1.86                     | 1.06              |
| 42:DH:12:PRO:HD3    | 42:DH:49:VAL:HG12  | 1.37                     | 1.06              |
| 10:AJ:48:THR:HA     | 10:AJ:62:HIS:HB3   | 1.35                     | 1.06              |
| 56:BX:11:PRO:HA     | 56:BX:28:PHE:HB3   | 1.36                     | 1.06              |
| 58:BZ:69:THR:HG22   | 58:BZ:90:VAL:HA    | 1.36                     | 1.06              |
| 51:DS:13:ARG:HG3    | 51:DS:14:VAL:H     | 1.16                     | 1.06              |
| 57:DY:76:CYS:SG     | 57:DY:77:PRO:HD2   | 1.95                     | 1.06              |
| 35:DA:1845:G:H2'    | 35:DA:1846:G:H5''  | 1.36                     | 1.06              |
| 2:AB:185:ILE:HG22   | 2:AB:199:TYR:HB2   | 1.31                     | 1.05              |
| 57:BY:28:LYS:HB3    | 57:BY:37:VAL:HB    | 1.31                     | 1.05              |
| 35:BA:1503:U:H2'    | 35:BA:1504:C:H6    | 1.15                     | 1.05              |
| 48:BP:55:ARG:HG2    | 48:BP:56:SER:H     | 1.17                     | 1.05              |
| 51:BS:13:ARG:HG3    | 51:BS:14:VAL:H     | 1.17                     | 1.05              |
| 38:DD:263:ARG:HB2   | 38:DD:263:ARG:NH1  | 1.70                     | 1.05              |
| 40:DF:40:GLN:HE22   | 40:DF:182:ASN:HB2  | 1.20                     | 1.05              |
| 57:DY:28:LYS:HB3    | 57:DY:37:VAL:HB    | 1.34                     | 1.05              |
| 42:BH:12:PRO:HD3    | 42:BH:49:VAL:HG12  | 1.37                     | 1.05              |
| 27:B2:69:ARG:HH22   | 35:BA:111:A:H4'    | 1.20                     | 1.05              |
| 35:BA:1747(A):G:C2' | 35:BA:1748:G:H5''  | 1.85                     | 1.05              |
| 31:D6:5:VAL:HG23    | 35:DA:2283:C:H5'   | 1.35                     | 1.05              |
| 5:CE:87:SER:HB3     | 5:CE:131:ILE:HD13  | 1.38                     | 1.05              |
| 24:CY:409:ILE:HG22  | 24:CY:459:LEU:HD21 | 1.37                     | 1.05              |
| 57:DY:7:VAL:HB      | 57:DY:8:LYS:HD2    | 1.37                     | 1.05              |
| 42:BH:157:TYR:CE1   | 42:BH:171:LEU:CD2  | 2.30                     | 1.05              |
| 56:DX:11:PRO:HA     | 56:DX:28:PHE:HB3   | 1.39                     | 1.05              |
| 1:AA:793:U:H3'      | 1:AA:794:A:H5''    | 1.36                     | 1.05              |
| 13:CM:27:LYS:HE2    | 13:CM:31:LYS:HE3   | 1.38                     | 1.05              |
| 41:DG:46:ALA:HB2    | 41:DG:88:ILE:HB    | 1.36                     | 1.05              |
| 35:BA:211:A:H2'     | 35:BA:212:G:H5''   | 1.33                     | 1.05              |
| 58:BZ:151:HIS:HA    | 58:BZ:171:ILE:HG23 | 1.36                     | 1.05              |
| 10:CJ:75:ILE:HG13   | 10:CJ:76:ASN:H     | 1.17                     | 1.05              |
| 40:DF:154:VAL:HG22  | 40:DF:191:ARG:HB3  | 1.35                     | 1.05              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 41:DG:62:LEU:HD12   | 41:DG:62:LEU:H     | 1.22                     | 1.05              |
| 10:CJ:48:THR:HA     | 10:CJ:62:HIS:HB3   | 1.32                     | 1.04              |
| 35:DA:1899:G:N2     | 35:DA:1902:C:H41   | 1.54                     | 1.04              |
| 38:BD:71:ASP:HB2    | 38:BD:103:ARG:HH22 | 1.20                     | 1.04              |
| 3:AC:70:VAL:HG12    | 3:AC:72:LYS:H      | 1.20                     | 1.04              |
| 48:DP:55:ARG:HG2    | 48:DP:56:SER:H     | 1.22                     | 1.04              |
| 57:BY:7:VAL:HB      | 57:BY:8:LYS:HD2    | 1.35                     | 1.04              |
| 24:CY:92:ILE:HG23   | 24:CY:93:GLU:H     | 1.22                     | 1.04              |
| 35:DA:1747(A):G:C2' | 35:DA:1748:G:H5''  | 1.87                     | 1.04              |
| 35:DA:965:C:H5'     | 35:DA:2273:A:H1'   | 1.40                     | 1.04              |
| 1:AA:1238:A:H5'     | 1:AA:1336:C:H41    | 1.19                     | 1.04              |
| 10:AJ:34:VAL:HG22   | 10:AJ:74:ILE:HG22  | 1.39                     | 1.04              |
| 52:BT:115:ARG:HB3   | 52:BT:115:ARG:HH11 | 1.23                     | 1.04              |
| 52:BT:65:LYS:HE3    | 52:BT:66:VAL:H     | 1.21                     | 1.04              |
| 38:DD:65:ILE:HG22   | 38:DD:104:TYR:HB3  | 1.40                     | 1.04              |
| 22:AV:21:A:H61      | 22:AV:46:G:H2'     | 1.20                     | 1.03              |
| 19:CS:50:ALA:HB1    | 19:CS:57:HIS:HB3   | 1.34                     | 1.03              |
| 23:CX:13:A:C3'      | 23:CX:14:A:H5''    | 1.87                     | 1.03              |
| 1:AA:1318:A:H1'     | 19:AS:37:ARG:HH21  | 1.18                     | 1.03              |
| 40:BF:167:ALA:HB1   | 40:BF:173:VAL:HG11 | 1.37                     | 1.03              |
| 57:DY:76:CYS:HB3    | 57:DY:96:ILE:HD11  | 1.40                     | 1.03              |
| 24:AY:662:LYS:HZ1   | 42:BH:175:LYS:HE3  | 1.07                     | 1.03              |
| 38:BD:65:ILE:HG22   | 38:BD:104:TYR:HB3  | 1.39                     | 1.03              |
| 35:BA:1899:G:N2     | 35:BA:1902:C:H41   | 1.55                     | 1.03              |
| 41:BG:77:ILE:HG22   | 41:BG:80:PHE:N     | 1.73                     | 1.03              |
| 35:DA:2579:C:H4'    | 39:DE:134:ILE:HG12 | 1.40                     | 1.03              |
| 3:AC:16:ARG:HH11    | 3:AC:16:ARG:HB2    | 1.23                     | 1.03              |
| 13:AM:27:LYS:HE2    | 13:AM:31:LYS:HE3   | 1.40                     | 1.03              |
| 25:B0:11:ARG:HB2    | 25:B0:11:ARG:HH11  | 1.18                     | 1.03              |
| 44:BK:115:LEU:HD22  | 44:BK:126:MET:HE2  | 1.41                     | 1.03              |
| 10:CJ:34:VAL:HG22   | 10:CJ:74:ILE:HG22  | 1.40                     | 1.03              |
| 5:AE:101:ILE:HD11   | 5:AE:119:LEU:HA    | 1.40                     | 1.03              |
| 1:CA:1003:G:H2'     | 1:CA:1004:A:H4'    | 1.37                     | 1.03              |
| 3:CC:70:VAL:HG12    | 3:CC:72:LYS:H      | 1.17                     | 1.03              |
| 35:DA:1452:A:H3'    | 35:DA:1453:U:H5''  | 1.36                     | 1.03              |
| 30:D5:44:THR:HG21   | 50:DR:101:ALA:HB2  | 1.41                     | 1.03              |
| 30:B5:2:ALA:HA      | 35:BA:2015:A:H1'   | 1.39                     | 1.03              |
| 38:DD:71:ASP:HB2    | 38:DD:103:ARG:HH22 | 1.17                     | 1.03              |
| 26:D1:44:PRO:HG2    | 26:D1:46:LEU:HD21  | 1.41                     | 1.02              |
| 35:DA:1503:U:H2'    | 35:DA:1504:C:H6    | 1.14                     | 1.02              |
| 24:AY:423:LYS:HB3   | 24:AY:472:VAL:HG22 | 1.41                     | 1.02              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 24:CY:17:ILE:O      | 24:CY:85:PRO:HG2   | 1.60                     | 1.02              |
| 40:DF:192:LEU:HD21  | 40:DF:194:MET:HG3  | 1.41                     | 1.02              |
| 41:DG:38:VAL:HG23   | 41:DG:158:ALA:HB3  | 1.38                     | 1.02              |
| 44:BK:19:PRO:HB3    | 44:BK:34:ILE:HD12  | 1.40                     | 1.02              |
| 57:BY:76:CYS:SG     | 57:BY:77:PRO:HD2   | 1.98                     | 1.02              |
| 52:DT:115:ARG:HH11  | 52:DT:115:ARG:HB3  | 1.24                     | 1.02              |
| 44:DK:19:PRO:HB3    | 44:DK:34:ILE:HD12  | 1.41                     | 1.02              |
| 30:D5:2:ALA:HA      | 35:DA:2015:A:H1'   | 1.39                     | 1.02              |
| 24:CY:136:ALA:HB3   | 24:CY:260:LEU:HB3  | 1.37                     | 1.02              |
| 37:DC:128:LEU:HD21  | 37:DC:132:LEU:HD11 | 1.41                     | 1.02              |
| 1:CA:1238:A:H5'     | 1:CA:1336:C:H41    | 1.22                     | 1.01              |
| 57:BY:76:CYS:HB3    | 57:BY:96:ILE:HD11  | 1.43                     | 1.01              |
| 12:AL:18:VAL:HG23   | 12:AL:19:ARG:H     | 1.24                     | 1.01              |
| 48:BP:41:ARG:HA     | 48:BP:41:ARG:HH21  | 1.25                     | 1.01              |
| 30:B5:44:THR:HG21   | 50:BR:101:ALA:HB2  | 1.42                     | 1.01              |
| 58:BZ:28:MET:HB3    | 58:BZ:88:PHE:HB2   | 1.42                     | 1.01              |
| 47:DO:111:PHE:HB3   | 47:DO:114:ILE:HD13 | 1.42                     | 1.01              |
| 22:CV:47:U:H3'      | 22:CV:48:C:H5'     | 1.38                     | 1.01              |
| 24:CY:84:THR:H      | 24:CY:85:PRO:HD3   | 1.25                     | 1.01              |
| 40:DF:8:GLN:HB3     | 40:DF:126:VAL:HA   | 1.42                     | 1.01              |
| 48:DP:41:ARG:HH21   | 48:DP:41:ARG:HA    | 1.25                     | 1.01              |
| 52:DT:28:VAL:HG21   | 52:DT:46:GLU:HG3   | 1.39                     | 1.01              |
| 41:BG:133:LEU:HD11  | 41:BG:157:ILE:HD12 | 1.42                     | 1.01              |
| 13:CM:124:PRO:HG2   | 24:CY:574:GLU:H    | 1.25                     | 1.01              |
| 1:AA:979:C:C3'      | 1:AA:980:C:H5''    | 1.90                     | 1.00              |
| 35:BA:2287:A:H62    | 35:BA:2344:U:H3    | 1.01                     | 1.00              |
| 24:CY:33:LEU:HD23   | 24:CY:360:ALA:HB2  | 1.40                     | 1.00              |
| 44:BK:4:VAL:HG12    | 44:BK:5:VAL:H      | 1.26                     | 1.00              |
| 35:DA:2287:A:H62    | 35:DA:2344:U:H3    | 1.01                     | 1.00              |
| 48:DP:16:ARG:HD3    | 48:DP:18:ARG:H     | 1.26                     | 1.00              |
| 3:CC:58:GLU:H       | 3:CC:65:ALA:HB3    | 1.26                     | 1.00              |
| 35:BA:1452:A:H3'    | 35:BA:1453:U:H5''  | 1.38                     | 1.00              |
| 35:DA:154(A):C:H5'' | 35:DA:155:U:H5''   | 1.44                     | 1.00              |
| 1:AA:1128:C:H2'     | 1:AA:1129:C:H5''   | 1.42                     | 1.00              |
| 5:CE:101:ILE:HD11   | 5:CE:119:LEU:HA    | 1.43                     | 1.00              |
| 2:AB:168:THR:HG23   | 2:AB:192:SER:HB3   | 1.38                     | 1.00              |
| 1:CA:1057:G:H5''    | 3:CC:154:SER:HB2   | 1.42                     | 1.00              |
| 44:DK:115:LEU:HD22  | 44:DK:126:MET:HE2  | 1.40                     | 1.00              |
| 1:CA:1489:G:C2'     | 1:CA:1490:C:H5''   | 1.91                     | 1.00              |
| 41:DG:68:PRO:HA     | 41:DG:92:VAL:CG1   | 1.92                     | 1.00              |
| 24:AY:546:ILE:HG23  | 24:AY:590:ILE:HG13 | 1.40                     | 1.00              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 2:CB:168:THR:HG23  | 2:CB:192:SER:HB3    | 1.40                     | 1.00              |
| 35:DA:1301:A:O2'   | 35:DA:1302:A:H2'    | 1.62                     | 1.00              |
| 35:BA:142:A:H1'    | 35:BA:1408:C:H1'    | 1.44                     | 0.99              |
| 1:CA:979:C:C3'     | 1:CA:980:C:H5''     | 1.92                     | 0.99              |
| 24:CY:153:MET:HA   | 24:CY:157:LEU:HD21  | 1.43                     | 0.99              |
| 25:D0:27:GLU:CD    | 25:D0:27:GLU:H      | 1.64                     | 0.99              |
| 31:B6:48:VAL:HG23  | 31:B6:49:HIS:H      | 1.27                     | 0.99              |
| 35:BA:2523:G:H2'   | 35:BA:2524:G:H5''   | 1.44                     | 0.99              |
| 38:BD:35:LYS:HD2   | 38:BD:36:PRO:N      | 1.77                     | 0.99              |
| 40:BF:40:GLN:HE22  | 40:BF:182:ASN:HB2   | 1.19                     | 0.99              |
| 52:BT:38:ASN:C     | 52:BT:38:ASN:HD22   | 1.65                     | 0.99              |
| 52:DT:65:LYS:HE3   | 52:DT:66:VAL:H      | 1.24                     | 0.99              |
| 25:B0:27:GLU:H     | 25:B0:27:GLU:CD     | 1.64                     | 0.99              |
| 54:BV:15:GLU:HB3   | 54:BV:16:PRO:HD2    | 1.42                     | 0.99              |
| 46:DN:54:VAL:HB    | 46:DN:122:VAL:HG22  | 1.43                     | 0.99              |
| 5:AE:80:ILE:HG22   | 8:AH:104:ARG:NH2    | 1.78                     | 0.99              |
| 40:DF:110:LEU:HD12 | 40:DF:206:ILE:HD11  | 1.43                     | 0.99              |
| 58:DZ:115:GLY:H    | 58:DZ:177:PRO:HG3   | 1.25                     | 0.99              |
| 5:AE:87:SER:HB3    | 5:AE:131:ILE:HD13   | 1.41                     | 0.99              |
| 18:AR:37:VAL:HG23  | 18:AR:38:GLU:H      | 1.27                     | 0.99              |
| 35:DA:2286:A:H4'   | 35:DA:2287:A:H5'    | 1.45                     | 0.99              |
| 52:DT:38:ASN:C     | 52:DT:38:ASN:HD22   | 1.65                     | 0.99              |
| 35:BA:2579:C:H4'   | 39:BE:134:ILE:HG12  | 1.44                     | 0.99              |
| 40:BF:8:GLN:HB3    | 40:BF:126:VAL:HA    | 1.41                     | 0.99              |
| 23:AX:13:A:C3'     | 23:AX:14:A:H5''     | 1.92                     | 0.99              |
| 38:DD:44:ASN:HB3   | 38:DD:49:ILE:HA     | 1.44                     | 0.99              |
| 35:BA:1452:A:H3'   | 35:BA:1453:U:C5'    | 1.92                     | 0.98              |
| 35:BA:272(G):C:H2' | 35:BA:272(H):C:H5'' | 1.44                     | 0.98              |
| 24:CY:546:ILE:HG23 | 24:CY:590:ILE:HG13  | 1.39                     | 0.98              |
| 48:BP:16:ARG:HD3   | 48:BP:18:ARG:H      | 1.28                     | 0.98              |
| 1:CA:1321:C:H3'    | 1:CA:1322:C:H5''    | 1.45                     | 0.98              |
| 35:DA:1452:A:H3'   | 35:DA:1453:U:C5'    | 1.92                     | 0.98              |
| 58:DZ:179:ASP:HB3  | 58:DZ:182:LYS:HE2   | 1.45                     | 0.98              |
| 12:AL:83:VAL:HG11  | 12:AL:100:ILE:HD13  | 1.44                     | 0.98              |
| 1:CA:975:A:H4'     | 1:CA:976:G:H5''     | 1.45                     | 0.98              |
| 12:CL:18:VAL:HG23  | 12:CL:19:ARG:H      | 1.26                     | 0.98              |
| 27:B2:3:LEU:HD22   | 27:B2:7:ARG:HH12    | 1.28                     | 0.98              |
| 38:BD:44:ASN:HB3   | 38:BD:49:ILE:HA     | 1.43                     | 0.98              |
| 35:DA:272(J):C:H3' | 35:DA:274:G:H5''    | 1.44                     | 0.98              |
| 41:BG:59:GLU:HA    | 41:BG:62:LEU:HD13   | 1.43                     | 0.98              |
| 35:DA:272(G):C:H2' | 35:DA:272(H):C:H5'' | 1.43                     | 0.98              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 24:AY:35:TYR:OH     | 24:AY:266:ASN:HB3  | 1.64                     | 0.98              |
| 40:BF:110:LEU:HD12  | 40:BF:206:ILE:HD11 | 1.46                     | 0.98              |
| 52:BT:28:VAL:HG21   | 52:BT:46:GLU:HG3   | 1.43                     | 0.98              |
| 38:BD:32:SER:O      | 38:BD:36:PRO:HG3   | 1.64                     | 0.98              |
| 24:CY:84:THR:HA     | 61:CY:702:FUA:H322 | 1.46                     | 0.98              |
| 38:DD:34:VAL:HG23   | 38:DD:35:LYS:H     | 1.28                     | 0.98              |
| 1:AA:975:A:H4'      | 1:AA:976:G:H5''    | 1.45                     | 0.97              |
| 28:B3:31:LEU:HD13   | 28:B3:32:GLN:HG2   | 1.44                     | 0.97              |
| 35:BA:1301:A:O2'    | 35:BA:1302:A:H2'   | 1.63                     | 0.97              |
| 53:BU:20:LEU:H      | 53:BU:20:LEU:HD22  | 1.29                     | 0.97              |
| 58:BZ:166:SER:HB2   | 58:BZ:167:PRO:C    | 1.83                     | 0.97              |
| 26:D1:76:ARG:HH22   | 26:D1:95:LEU:HD13  | 1.26                     | 0.97              |
| 35:DA:211:A:C2'     | 35:DA:212:G:H5''   | 1.93                     | 0.97              |
| 39:DE:38:THR:HG22   | 39:DE:40:GLU:H     | 1.25                     | 0.97              |
| 35:BA:2262:U:H2'    | 35:BA:2263:C:H5'   | 1.46                     | 0.97              |
| 35:DA:612:C:C2'     | 35:DA:613:G:H5''   | 1.94                     | 0.97              |
| 44:DK:93:ARG:HB2    | 58:DZ:112:ARG:HE   | 1.25                     | 0.97              |
| 24:AY:276:VAL:HA    | 24:AY:280:LEU:HD23 | 1.44                     | 0.97              |
| 47:BO:111:PHE:HB3   | 47:BO:114:ILE:HD13 | 1.46                     | 0.97              |
| 35:DA:1803:A:O3'    | 38:DD:259:THR:HG21 | 1.64                     | 0.97              |
| 24:AY:428:LEU:HD13  | 24:AY:440:VAL:HG11 | 1.42                     | 0.97              |
| 33:B8:33:ASN:H      | 33:B8:33:ASN:ND2   | 1.61                     | 0.97              |
| 35:BA:154(A):C:H5'' | 35:BA:155:U:H5''   | 1.45                     | 0.97              |
| 46:BN:48:MET:H      | 46:BN:48:MET:HE2   | 1.25                     | 0.97              |
| 28:D3:31:LEU:HD13   | 28:D3:32:GLN:HG2   | 1.44                     | 0.97              |
| 31:D6:48:VAL:HG23   | 31:D6:49:HIS:H     | 1.30                     | 0.97              |
| 35:BA:2286:A:H4'    | 35:BA:2287:A:H5'   | 1.44                     | 0.97              |
| 22:CW:21:U:O2'      | 35:DA:2112:G:H1'   | 1.64                     | 0.97              |
| 3:AC:58:GLU:H       | 3:AC:65:ALA:HB3    | 1.28                     | 0.97              |
| 35:BA:1814:G:H3'    | 35:BA:1815:A:H5''  | 1.46                     | 0.97              |
| 35:BA:211:A:C2'     | 35:BA:212:G:H5''   | 1.94                     | 0.97              |
| 22:AV:46:G:H4'      | 22:AV:47:U:H5      | 1.25                     | 0.97              |
| 24:AY:427:ALA:HB1   | 24:AY:466:LEU:HD11 | 1.44                     | 0.97              |
| 28:D3:17:LYS:HG2    | 35:DA:969:U:OP1    | 1.65                     | 0.97              |
| 3:AC:52:LEU:HD23    | 3:AC:52:LEU:H      | 1.30                     | 0.97              |
| 18:CR:37:VAL:HG23   | 18:CR:38:GLU:H     | 1.25                     | 0.97              |
| 24:AY:84:THR:H      | 24:AY:85:PRO:HD2   | 1.27                     | 0.96              |
| 3:CC:16:ARG:HB2     | 3:CC:16:ARG:HH11   | 1.26                     | 0.96              |
| 35:DA:2523:G:H2'    | 35:DA:2524:G:H5''  | 1.44                     | 0.96              |
| 39:DE:117:MET:HA    | 39:DE:122:PHE:H    | 1.30                     | 0.96              |
| 1:CA:686:U:HO2'     | 1:CA:687:A:H8      | 0.97                     | 0.96              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:D2:16:LEU:HB3   | 27:D2:20:GLU:HG2   | 1.45                     | 0.96              |
| 1:AA:129(A):G:O2'  | 1:AA:189(F):U:H2'  | 1.66                     | 0.96              |
| 24:AY:409:ILE:HD11 | 24:AY:654:GLY:HA2  | 1.44                     | 0.96              |
| 1:CA:1128:C:H2'    | 1:CA:1129:C:H5''   | 1.43                     | 0.96              |
| 51:DS:15:ARG:HB3   | 51:DS:18:ILE:HD11  | 1.47                     | 0.96              |
| 35:DA:27:G:H22     | 35:DA:512:G:H2'    | 1.29                     | 0.96              |
| 47:DO:17:ARG:HE    | 47:DO:47:ILE:HD11  | 1.30                     | 0.96              |
| 39:BE:38:THR:HG22  | 39:BE:40:GLU:H     | 1.25                     | 0.96              |
| 25:B0:7:LEU:HD12   | 49:BQ:85:LYS:HE2   | 1.47                     | 0.96              |
| 5:CE:50:GLU:HG3    | 5:CE:52:PRO:HD2    | 1.46                     | 0.96              |
| 38:DD:32:SER:O     | 38:DD:36:PRO:HG3   | 1.66                     | 0.96              |
| 1:AA:1057:G:H5''   | 3:AC:154:SER:HB2   | 1.44                     | 0.96              |
| 44:DK:99:ILE:HG23  | 44:DK:103:GLN:HB2  | 1.47                     | 0.96              |
| 24:AY:453:GLY:HA3  | 24:AY:459:LEU:HD11 | 1.46                     | 0.96              |
| 35:BA:27:G:H22     | 35:BA:512:G:H2'    | 1.30                     | 0.96              |
| 40:DF:3:GLU:CA     | 40:DF:24:LEU:HG    | 1.95                     | 0.96              |
| 35:DA:240:G:H3'    | 35:DA:241:A:H5''   | 1.45                     | 0.96              |
| 51:DS:28:VAL:HG12  | 51:DS:29:PHE:H     | 1.31                     | 0.96              |
| 35:BA:612:C:C2'    | 35:BA:613:G:H5''   | 1.95                     | 0.96              |
| 4:CD:129:ASN:HD21  | 4:CD:145:GLU:H     | 1.13                     | 0.96              |
| 38:DD:35:LYS:HD2   | 38:DD:36:PRO:N     | 1.81                     | 0.96              |
| 1:AA:1321:C:H3'    | 1:AA:1322:C:H5''   | 1.45                     | 0.95              |
| 28:B3:16:PRO:HB2   | 28:B3:18:ASP:OD1   | 1.65                     | 0.95              |
| 35:BA:272(J):C:H3' | 35:BA:274:G:H5''   | 1.45                     | 0.95              |
| 2:CB:118:LEU:HB3   | 2:CB:142:LEU:HD12  | 1.47                     | 0.95              |
| 22:CV:17:C:H5''    | 22:CV:17(A):U:H6   | 1.30                     | 0.95              |
| 35:DA:2584:U:H2'   | 35:DA:2585:U:H5'   | 1.48                     | 0.95              |
| 48:DP:30:THR:HG22  | 48:DP:31:ALA:H     | 1.30                     | 0.95              |
| 48:BP:38:GLN:HG3   | 48:BP:39:LYS:H     | 1.31                     | 0.95              |
| 48:DP:59:LEU:HA    | 48:DP:61:ARG:NE    | 1.81                     | 0.95              |
| 38:BD:34:VAL:HG23  | 38:BD:35:LYS:H     | 1.30                     | 0.95              |
| 41:BG:135:LEU:HD11 | 41:BG:155:MET:HG2  | 1.46                     | 0.95              |
| 33:D8:61:LEU:HD12  | 33:D8:62:LEU:H     | 1.31                     | 0.95              |
| 26:B1:86:SER:HB3   | 26:B1:89:GLU:HB2   | 1.46                     | 0.95              |
| 26:B1:81:LYS:HE2   | 35:BA:271(H):G:H4' | 1.48                     | 0.95              |
| 46:BN:46:VAL:HG13  | 46:BN:47:ALA:H     | 1.30                     | 0.95              |
| 1:CA:1452:C:H1'    | 1:CA:1456:G:N2     | 1.81                     | 0.95              |
| 35:DA:142:A:H1'    | 35:DA:1408:C:H1'   | 1.45                     | 0.95              |
| 26:D1:46:LEU:HD22  | 26:D1:46:LEU:H     | 1.30                     | 0.95              |
| 35:BA:1884:A:H2'   | 35:BA:1885:A:H5''  | 1.48                     | 0.95              |
| 48:BP:59:LEU:HA    | 48:BP:61:ARG:NE    | 1.80                     | 0.95              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:1884:A:H2'   | 35:DA:1885:A:H5''  | 1.47                     | 0.95              |
| 46:DN:48:MET:H     | 46:DN:48:MET:HE2   | 1.27                     | 0.95              |
| 35:BA:2584:U:H2'   | 35:BA:2585:U:H5'   | 1.47                     | 0.95              |
| 46:BN:54:VAL:HB    | 46:BN:122:VAL:HG22 | 1.46                     | 0.95              |
| 24:CY:388:THR:HG21 | 24:CY:399:LEU:HD13 | 1.49                     | 0.95              |
| 35:DA:2310:A:O2'   | 35:DA:2311:A:H5'   | 1.67                     | 0.95              |
| 1:AA:1489:G:H2'    | 1:AA:1490:C:H5''   | 1.47                     | 0.95              |
| 1:AA:80:G:H3'      | 1:AA:81:U:H5'      | 1.48                     | 0.95              |
| 48:BP:30:THR:HG22  | 48:BP:31:ALA:H     | 1.30                     | 0.95              |
| 27:D2:69:ARG:HH22  | 35:DA:111:A:H5''   | 1.32                     | 0.95              |
| 28:D3:16:PRO:HB2   | 28:D3:18:ASP:OD1   | 1.67                     | 0.95              |
| 35:DA:2572:A:H5'   | 35:DA:2574:G:H4'   | 1.49                     | 0.95              |
| 48:DP:38:GLN:HG3   | 48:DP:39:LYS:H     | 1.27                     | 0.95              |
| 1:AA:1502:A:H2     | 1:AA:1505:G:H1     | 0.98                     | 0.95              |
| 40:BF:84:VAL:HG12  | 40:BF:85:GLY:N     | 1.82                     | 0.95              |
| 48:DP:85:LEU:HD12  | 48:DP:120:ALA:HB2  | 1.49                     | 0.95              |
| 40:BF:192:LEU:HD21 | 40:BF:194:MET:HG3  | 1.44                     | 0.94              |
| 40:BF:34:TRP:HB2   | 48:BP:10:PRO:HB2   | 1.46                     | 0.94              |
| 38:DD:35:LYS:HG2   | 38:DD:63:ARG:HA    | 1.49                     | 0.94              |
| 53:DU:20:LEU:H     | 53:DU:20:LEU:HD22  | 1.31                     | 0.94              |
| 6:AF:37:VAL:HG12   | 6:AF:38:GLU:H      | 1.32                     | 0.94              |
| 35:BA:1803:A:O3'   | 38:BD:259:THR:HG21 | 1.67                     | 0.94              |
| 50:BR:99:LYS:N     | 50:BR:99:LYS:HD3   | 1.83                     | 0.94              |
| 51:BS:34:HIS:HB3   | 51:BS:53:SER:HB3   | 1.49                     | 0.94              |
| 50:DR:99:LYS:HD3   | 50:DR:99:LYS:N     | 1.82                     | 0.94              |
| 35:DA:813:U:H2'    | 35:DA:814:C:C6     | 2.02                     | 0.94              |
| 35:BA:1503:U:H2'   | 35:BA:1504:C:C6    | 2.02                     | 0.94              |
| 6:CF:37:VAL:HG12   | 6:CF:38:GLU:H      | 1.29                     | 0.94              |
| 33:D8:33:ASN:H     | 33:D8:33:ASN:HD22  | 0.97                     | 0.94              |
| 44:DK:106:GLU:HA   | 44:DK:109:LYS:HD3  | 1.50                     | 0.94              |
| 33:B8:61:LEU:HD12  | 33:B8:62:LEU:H     | 1.32                     | 0.94              |
| 54:DV:15:GLU:HB3   | 54:DV:16:PRO:HD2   | 1.45                     | 0.94              |
| 1:AA:1128:C:C2'    | 1:AA:1129:C:H5''   | 1.98                     | 0.94              |
| 11:AK:54:ARG:O     | 11:AK:57:THR:HG22  | 1.68                     | 0.94              |
| 35:BA:1038:C:H3'   | 35:BA:1039:G:H5''  | 1.50                     | 0.94              |
| 35:BA:240:G:H3'    | 35:BA:241:A:H5''   | 1.49                     | 0.94              |
| 39:BE:116:VAL:O    | 39:BE:117:MET:HB3  | 1.63                     | 0.94              |
| 1:CA:129(A):G:O2'  | 1:CA:189(F):U:H2'  | 1.67                     | 0.94              |
| 35:DA:1038:C:H3'   | 35:DA:1039:G:H5''  | 1.49                     | 0.94              |
| 35:DA:2133:G:H2'   | 35:DA:2157:G:N2    | 1.83                     | 0.94              |
| 48:BP:85:LEU:HD12  | 48:BP:120:ALA:HB2  | 1.48                     | 0.94              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:1503:U:H2'   | 35:DA:1504:C:C6    | 2.01                     | 0.94              |
| 36:BB:7:G:H2'      | 36:BB:8:U:H5''     | 1.49                     | 0.94              |
| 20:AT:13:LEU:HD12  | 20:AT:13:LEU:H     | 1.33                     | 0.94              |
| 2:CB:44:LEU:H      | 2:CB:44:LEU:HD12   | 1.31                     | 0.94              |
| 39:DE:116:VAL:O    | 39:DE:117:MET:HB3  | 1.67                     | 0.94              |
| 48:DP:7:ARG:HB3    | 48:DP:8:PRO:HD3    | 1.50                     | 0.94              |
| 56:DX:12:VAL:HG23  | 56:DX:13:LEU:N     | 1.81                     | 0.94              |
| 26:B1:46:LEU:HB3   | 26:B1:63:ALA:HA    | 1.46                     | 0.94              |
| 35:BA:2310:A:O2'   | 35:BA:2311:A:H5'   | 1.68                     | 0.94              |
| 1:AA:686:U:HO2'    | 1:AA:687:A:H8      | 0.98                     | 0.93              |
| 51:BS:28:VAL:HG12  | 51:BS:29:PHE:H     | 1.31                     | 0.93              |
| 30:D5:56:LYS:HG3   | 30:D5:57:VAL:H     | 1.33                     | 0.93              |
| 35:DA:1814:G:H3'   | 35:DA:1815:A:H5''  | 1.48                     | 0.93              |
| 58:DZ:7:ALA:HB3    | 58:DZ:61:LEU:HD23  | 1.50                     | 0.93              |
| 17:AQ:69:LYS:O     | 17:AQ:70:ARG:HD2   | 1.68                     | 0.93              |
| 44:BK:6:ALA:HB3    | 44:BK:59:ILE:HG22  | 1.47                     | 0.93              |
| 44:BK:99:ILE:HG23  | 44:BK:103:GLN:HB2  | 1.48                     | 0.93              |
| 1:CA:1128:C:C2'    | 1:CA:1129:C:H5''   | 1.98                     | 0.93              |
| 26:D1:23:LYS:HE2   | 26:D1:28:GLY:HA3   | 1.49                     | 0.93              |
| 41:DG:60:LEU:HA    | 41:DG:63:ILE:HD11  | 1.50                     | 0.93              |
| 46:DN:46:VAL:HG13  | 46:DN:47:ALA:H     | 1.31                     | 0.93              |
| 35:DA:871:U:OP1    | 49:DQ:5:ARG:HG3    | 1.69                     | 0.93              |
| 52:DT:28:VAL:HG22  | 52:DT:46:GLU:HA    | 1.48                     | 0.93              |
| 58:DZ:29:TYR:HB3   | 58:DZ:34:ASN:HB2   | 1.50                     | 0.93              |
| 3:AC:20:SER:HB3    | 3:AC:40:ARG:HH22   | 1.33                     | 0.93              |
| 38:BD:35:LYS:HG2   | 38:BD:63:ARG:HA    | 1.49                     | 0.93              |
| 51:BS:15:ARG:HB3   | 51:BS:18:ILE:HD11  | 1.50                     | 0.93              |
| 3:CC:52:LEU:HD23   | 3:CC:52:LEU:H      | 1.34                     | 0.93              |
| 35:DA:2756:U:H4'   | 35:DA:2757:A:OP1   | 1.68                     | 0.93              |
| 56:DX:35:THR:HG22  | 56:DX:37:THR:H     | 1.33                     | 0.93              |
| 2:AB:118:LEU:HB3   | 2:AB:142:LEU:HD12  | 1.49                     | 0.93              |
| 35:BA:2133:G:H2'   | 35:BA:2157:G:N2    | 1.82                     | 0.93              |
| 35:BA:2811:G:OP1   | 39:BE:60:ASN:HB2   | 1.69                     | 0.93              |
| 40:BF:3:GLU:CA     | 40:BF:24:LEU:HG    | 1.96                     | 0.93              |
| 46:BN:45:ASN:HD22  | 46:BN:45:ASN:H     | 1.12                     | 0.93              |
| 41:DG:133:LEU:HD12 | 41:DG:157:ILE:HB   | 1.49                     | 0.93              |
| 48:BP:55:ARG:HG2   | 48:BP:56:SER:N     | 1.79                     | 0.93              |
| 3:CC:70:VAL:HG12   | 3:CC:71:ALA:H      | 1.33                     | 0.93              |
| 12:CL:83:VAL:HG11  | 12:CL:100:ILE:HD13 | 1.47                     | 0.93              |
| 35:DA:2811:G:OP1   | 39:DE:60:ASN:HB2   | 1.68                     | 0.93              |
| 13:CM:49:THR:HG22  | 13:CM:51:ALA:H     | 1.34                     | 0.93              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:1899:G:H22   | 35:DA:1902:C:N4    | 1.66                     | 0.93              |
| 38:BD:263:ARG:CB   | 38:BD:263:ARG:HH11 | 1.80                     | 0.93              |
| 44:BK:106:GLU:HA   | 44:BK:109:LYS:HD3  | 1.49                     | 0.93              |
| 57:BY:8:LYS:HB2    | 57:BY:28:LYS:NZ    | 1.84                     | 0.93              |
| 3:CC:79:ARG:HH11   | 3:CC:79:ARG:HB2    | 1.32                     | 0.93              |
| 41:DG:63:ILE:HA    | 41:DG:143:GLU:HG3  | 1.51                     | 0.93              |
| 57:DY:8:LYS:HB2    | 57:DY:28:LYS:NZ    | 1.83                     | 0.93              |
| 19:AS:42:PRO:HB3   | 29:B4:50:VAL:HG21  | 1.51                     | 0.93              |
| 35:BA:2756:U:H4'   | 35:BA:2757:A:OP1   | 1.66                     | 0.93              |
| 24:CY:157:LEU:HD23 | 24:CY:157:LEU:H    | 1.32                     | 0.93              |
| 33:D8:56:GLU:HA    | 33:D8:59:LYS:NZ    | 1.83                     | 0.93              |
| 28:B3:17:LYS:HG2   | 35:BA:969:U:OP1    | 1.68                     | 0.93              |
| 39:BE:111:ARG:HA   | 50:BR:2:ARG:HB3    | 1.50                     | 0.93              |
| 52:BT:28:VAL:HG22  | 52:BT:46:GLU:HA    | 1.50                     | 0.93              |
| 35:BA:2245:U:H5'   | 35:BA:2246:G:H5'   | 1.51                     | 0.92              |
| 35:DA:1494:A:O2'   | 35:DA:1495:A:H5''  | 1.67                     | 0.92              |
| 35:DA:1845:G:C2'   | 35:DA:1846:G:H5''  | 1.99                     | 0.92              |
| 38:DD:70:TRP:CH2   | 38:DD:150:LYS:HA   | 2.04                     | 0.92              |
| 40:DF:34:TRP:HB2   | 48:DP:10:PRO:HB2   | 1.49                     | 0.92              |
| 40:DF:84:VAL:HG12  | 40:DF:85:GLY:N     | 1.82                     | 0.92              |
| 35:BA:1899:G:H22   | 35:BA:1902:C:N4    | 1.67                     | 0.92              |
| 48:BP:146:VAL:HG22 | 48:BP:147:LEU:H    | 1.33                     | 0.92              |
| 48:BP:7:ARG:HB3    | 48:BP:8:PRO:HD3    | 1.50                     | 0.92              |
| 4:CD:129:ASN:ND2   | 4:CD:145:GLU:H     | 1.66                     | 0.92              |
| 18:AR:29:PHE:HD2   | 18:AR:29:PHE:H     | 1.18                     | 0.92              |
| 35:BA:2572:A:H5'   | 35:BA:2574:G:H4'   | 1.47                     | 0.92              |
| 56:BX:12:VAL:HG23  | 56:BX:13:LEU:N     | 1.81                     | 0.92              |
| 24:CY:632:LEU:HG   | 24:CY:645:ALA:HA   | 1.51                     | 0.92              |
| 28:D3:8:LEU:HD22   | 28:D3:31:LEU:HD23  | 1.50                     | 0.92              |
| 35:DA:358:U:H2'    | 35:DA:359:A:H8     | 1.35                     | 0.92              |
| 48:DP:126:VAL:HA   | 48:DP:145:PRO:HB2  | 1.52                     | 0.92              |
| 48:DP:146:VAL:HG22 | 48:DP:147:LEU:H    | 1.31                     | 0.92              |
| 1:AA:1054:C:O2'    | 1:AA:1055:A:H5''   | 1.70                     | 0.92              |
| 11:AK:111:ASP:HA   | 18:AR:84:LYS:HD2   | 1.50                     | 0.92              |
| 35:BA:903:C:C2'    | 35:BA:904:C:H5''   | 1.99                     | 0.92              |
| 1:CA:973:G:H1'     | 10:CJ:55:LYS:NZ    | 1.83                     | 0.92              |
| 35:DA:2591:C:H2'   | 35:DA:2592:G:C8    | 2.05                     | 0.92              |
| 39:DE:107:THR:O    | 39:DE:190:GLY:HA2  | 1.67                     | 0.92              |
| 3:AC:70:VAL:HG12   | 3:AC:71:ALA:H      | 1.31                     | 0.92              |
| 35:BA:2591:C:H2'   | 35:BA:2592:G:C8    | 2.05                     | 0.92              |
| 56:BX:12:VAL:CG2   | 56:BX:13:LEU:H     | 1.83                     | 0.92              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 13:AM:49:THR:HG22   | 13:AM:51:ALA:H     | 1.33                     | 0.92              |
| 24:AY:415:PRO:HA    | 24:AY:474:ALA:HB2  | 1.50                     | 0.92              |
| 35:BA:1845:G:C2'    | 35:BA:1846:G:H5''  | 1.99                     | 0.92              |
| 52:BT:27:THR:O      | 52:BT:28:VAL:HG23  | 1.68                     | 0.92              |
| 35:DA:1348:G:H2'    | 35:DA:1349:A:H5''  | 1.52                     | 0.92              |
| 39:DE:47:VAL:HG12   | 39:DE:48:GLN:H     | 1.32                     | 0.92              |
| 25:D0:7:LEU:HD12    | 49:DQ:85:LYS:HE2   | 1.47                     | 0.92              |
| 35:BA:1494:A:O2'    | 35:BA:1495:A:H5''  | 1.69                     | 0.92              |
| 35:BA:1142(A):A:C2' | 35:BA:1143:A:H5''  | 1.99                     | 0.92              |
| 39:BE:117:MET:HA    | 39:BE:122:PHE:H    | 1.35                     | 0.92              |
| 39:BE:47:VAL:HG12   | 39:BE:48:GLN:H     | 1.33                     | 0.92              |
| 26:D1:76:ARG:HH12   | 26:D1:95:LEU:HD22  | 1.33                     | 0.92              |
| 35:DA:2262:U:H2'    | 35:DA:2263:C:H5'   | 1.49                     | 0.92              |
| 35:DA:903:C:C2'     | 35:DA:904:C:H5''   | 1.99                     | 0.92              |
| 58:DZ:151:HIS:HA    | 58:DZ:171:ILE:HG23 | 1.49                     | 0.92              |
| 3:AC:79:ARG:HB2     | 3:AC:79:ARG:HH11   | 1.32                     | 0.92              |
| 39:BE:33:VAL:HG12   | 39:BE:90:THR:H     | 1.35                     | 0.92              |
| 47:BO:17:ARG:HE     | 47:BO:47:ILE:HD11  | 1.30                     | 0.92              |
| 1:AA:1452:C:H1'     | 1:AA:1456:G:N2     | 1.84                     | 0.91              |
| 2:AB:165:VAL:HG23   | 2:AB:166:ASP:H     | 1.33                     | 0.91              |
| 1:CA:1054:C:O2'     | 1:CA:1055:A:H5''   | 1.69                     | 0.91              |
| 11:CK:54:ARG:O      | 11:CK:57:THR:HG22  | 1.68                     | 0.91              |
| 41:DG:121:ASN:HB3   | 41:DG:124:SER:HB2  | 1.52                     | 0.91              |
| 26:B1:80:LEU:HD23   | 26:B1:81:LYS:H     | 1.35                     | 0.91              |
| 33:B8:33:ASN:H      | 33:B8:33:ASN:HD22  | 0.99                     | 0.91              |
| 33:B8:56:GLU:HA     | 33:B8:59:LYS:NZ    | 1.83                     | 0.91              |
| 35:BA:1043:C:C2'    | 35:BA:1044:G:H5''  | 1.99                     | 0.91              |
| 35:BA:2296:U:H4'    | 35:BA:2297:C:OP1   | 1.70                     | 0.91              |
| 2:CB:204:ASN:ND2    | 2:CB:206:ASP:H     | 1.67                     | 0.91              |
| 24:AY:9:LEU:HD21    | 24:AY:284:LEU:HB2  | 1.49                     | 0.91              |
| 35:BA:2712:U:O2'    | 35:BA:2712(A):A:H8 | 1.53                     | 0.91              |
| 38:BD:70:TRP:CH2    | 38:BD:150:LYS:HA   | 2.05                     | 0.91              |
| 54:BV:51:VAL:HG12   | 54:BV:52:VAL:H     | 1.34                     | 0.91              |
| 1:CA:80:G:H3'       | 1:CA:81:U:H5'      | 1.48                     | 0.91              |
| 35:DA:2138:C:H2'    | 35:DA:2139:C:H6    | 1.33                     | 0.91              |
| 36:DB:7:G:H2'       | 36:DB:8:U:H5''     | 1.52                     | 0.91              |
| 35:DA:1203:G:H4'    | 48:DP:7:ARG:HD2    | 1.49                     | 0.91              |
| 51:DS:24:LEU:HB3    | 51:DS:85:VAL:HG12  | 1.52                     | 0.91              |
| 54:DV:51:VAL:HG12   | 54:DV:52:VAL:H     | 1.34                     | 0.91              |
| 24:AY:513:LYS:HB2   | 24:AY:566:THR:HB   | 1.52                     | 0.91              |
| 26:B1:76:ARG:HH12   | 26:B1:95:LEU:HD22  | 1.33                     | 0.91              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 35:BA:1020:A:N1     | 35:BA:1141:U:H2'   | 1.86                     | 0.91              |
| 31:D6:8:LYS:HE3     | 31:D6:25:LYS:HD3   | 1.50                     | 0.91              |
| 52:DT:23:ARG:HG2    | 52:DT:120:ARG:HH12 | 1.33                     | 0.91              |
| 10:AJ:55:LYS:H      | 10:AJ:55:LYS:CE    | 1.83                     | 0.91              |
| 24:AY:238:THR:HG22  | 24:AY:241:GLU:HG2  | 1.50                     | 0.91              |
| 44:DK:77:LEU:HD12   | 44:DK:107:ILE:HG23 | 1.52                     | 0.91              |
| 53:DU:90:VAL:HG21   | 54:DV:47:VAL:HG21  | 1.50                     | 0.91              |
| 35:BA:2138:C:H2'    | 35:BA:2139:C:H6    | 1.33                     | 0.91              |
| 42:BH:157:TYR:HE1   | 42:BH:171:LEU:HD21 | 1.34                     | 0.91              |
| 56:BX:35:THR:HG22   | 56:BX:37:THR:H     | 1.36                     | 0.91              |
| 1:CA:1356:G:H2'     | 1:CA:1357:A:C8     | 2.06                     | 0.91              |
| 35:DA:1142(A):A:C2' | 35:DA:1143:A:H5''  | 2.00                     | 0.91              |
| 35:DA:2296:U:H4'    | 35:DA:2297:C:OP1   | 1.68                     | 0.91              |
| 56:DX:12:VAL:CG2    | 56:DX:13:LEU:H     | 1.82                     | 0.91              |
| 1:AA:483:C:H3'      | 1:AA:484:G:H5''    | 1.52                     | 0.91              |
| 46:BN:133:GLN:HG2   | 46:BN:135:PRO:HD3  | 1.52                     | 0.91              |
| 1:CA:1251:A:H2'     | 1:CA:1252:A:C8     | 2.05                     | 0.91              |
| 35:DA:2110:G:O2'    | 35:DA:2120:G:H5'   | 1.71                     | 0.91              |
| 41:DG:34:LEU:HD22   | 41:DG:99:MET:HE3   | 1.52                     | 0.91              |
| 52:DT:23:ARG:O      | 52:DT:25:GLY:N     | 2.04                     | 0.91              |
| 44:BK:77:LEU:HD12   | 44:BK:107:ILE:HG23 | 1.53                     | 0.91              |
| 38:DD:263:ARG:CB    | 38:DD:263:ARG:HH11 | 1.82                     | 0.91              |
| 42:DH:157:TYR:HE1   | 42:DH:171:LEU:HD21 | 1.35                     | 0.91              |
| 30:B5:56:LYS:HG3    | 30:B5:57:VAL:H     | 1.33                     | 0.91              |
| 31:B6:8:LYS:HE3     | 31:B6:25:LYS:HD3   | 1.51                     | 0.91              |
| 39:BE:107:THR:O     | 39:BE:190:GLY:HA2  | 1.71                     | 0.91              |
| 24:CY:181:LEU:HD21  | 24:CY:243:VAL:HG22 | 1.51                     | 0.91              |
| 35:DA:1452:A:C3'    | 35:DA:1453:U:H5''  | 2.01                     | 0.91              |
| 52:DT:27:THR:O      | 52:DT:28:VAL:HG23  | 1.71                     | 0.91              |
| 58:DZ:20:ARG:HH11   | 58:DZ:20:ARG:HB2   | 1.33                     | 0.91              |
| 1:AA:973:G:H1'      | 10:AJ:55:LYS:NZ    | 1.85                     | 0.90              |
| 35:DA:1846:G:H8     | 35:DA:1846:G:H5'   | 1.33                     | 0.90              |
| 27:B2:41:ILE:HD11   | 27:B2:44:LEU:HD12  | 1.54                     | 0.90              |
| 35:BA:871:U:OP1     | 49:BQ:5:ARG:HG3    | 1.70                     | 0.90              |
| 52:BT:23:ARG:HG2    | 52:BT:120:ARG:HH12 | 1.34                     | 0.90              |
| 26:B1:86:SER:O      | 26:B1:90:ILE:HG12  | 1.71                     | 0.90              |
| 56:BX:24:GLY:O      | 56:BX:82:GLN:HA    | 1.72                     | 0.90              |
| 35:DA:2712:U:O2'    | 35:DA:2712(A):A:H8 | 1.54                     | 0.90              |
| 40:DF:170:LEU:HB2   | 40:DF:173:VAL:HB   | 1.52                     | 0.90              |
| 48:DP:39:LYS:HE2    | 48:DP:40:SER:H     | 1.37                     | 0.90              |
| 30:B5:4:HIS:HB3     | 30:B5:5:PRO:HD3    | 1.50                     | 0.90              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:CA:939:G:H5''     | 7:CG:102:ARG:NH2    | 1.86                     | 0.90              |
| 37:DC:128:LEU:HD21  | 37:DC:132:LEU:CD1   | 2.00                     | 0.90              |
| 58:DZ:151:HIS:HB3   | 58:DZ:170:THR:HA    | 1.54                     | 0.90              |
| 19:AS:41:VAL:HG21   | 19:AS:44:MET:HB2    | 1.53                     | 0.90              |
| 35:BA:1846:G:H5'    | 35:BA:1846:G:H8     | 1.34                     | 0.90              |
| 48:BP:126:VAL:HA    | 48:BP:145:PRO:HB2   | 1.52                     | 0.90              |
| 1:AA:1502:A:H2      | 1:AA:1505:G:N1      | 1.70                     | 0.90              |
| 53:BU:90:VAL:HG21   | 54:BV:47:VAL:HG21   | 1.49                     | 0.90              |
| 35:DA:2189:U:H2'    | 35:DA:2190:G:H5''   | 1.54                     | 0.90              |
| 46:DN:133:GLN:HG2   | 46:DN:135:PRO:HD3   | 1.52                     | 0.90              |
| 50:DR:100:LEU:HD22  | 50:DR:100:LEU:H     | 1.37                     | 0.90              |
| 51:DS:34:HIS:HB3    | 51:DS:53:SER:HB3    | 1.51                     | 0.90              |
| 3:AC:90:GLU:O       | 3:AC:93:LYS:HB3     | 1.72                     | 0.90              |
| 26:B1:45:ASN:HB2    | 35:BA:2230:G:H1'    | 1.54                     | 0.90              |
| 35:BA:654(M):C:HO2' | 35:BA:654(N):G:H8   | 0.94                     | 0.90              |
| 1:CA:979:C:H3'      | 1:CA:980:C:C5'      | 2.01                     | 0.90              |
| 20:CT:23:ARG:O      | 20:CT:27:LYS:HB2    | 1.72                     | 0.90              |
| 35:DA:1070:A:H5'    | 35:DA:1072:C:OP2    | 1.71                     | 0.90              |
| 35:DA:1020:A:N1     | 35:DA:1141:U:H2'    | 1.86                     | 0.90              |
| 50:DR:45:ARG:HG3    | 50:DR:46:GLY:H      | 1.35                     | 0.90              |
| 1:AA:979:C:H3'      | 1:AA:980:C:C5'      | 2.00                     | 0.90              |
| 50:BR:38:VAL:HB     | 50:BR:39:PRO:HD3    | 1.53                     | 0.90              |
| 35:DA:996:A:H4'     | 53:DU:92:ARG:NE     | 1.87                     | 0.90              |
| 24:AY:113:GLY:C     | 24:AY:115:GLU:H     | 1.75                     | 0.90              |
| 35:BA:2523:G:C2'    | 35:BA:2524:G:H5''   | 2.02                     | 0.90              |
| 44:BK:7:VAL:O       | 44:BK:7:VAL:HG13    | 1.72                     | 0.90              |
| 35:DA:1043:C:C2'    | 35:DA:1044:G:H5''   | 2.00                     | 0.90              |
| 54:DV:18:LEU:HD22   | 54:DV:19:LYS:H      | 1.35                     | 0.90              |
| 1:AA:720:C:H3'      | 1:AA:721:G:H5''     | 1.51                     | 0.90              |
| 10:AJ:50:ILE:H      | 10:AJ:50:ILE:HD13   | 1.34                     | 0.90              |
| 35:BA:1203:G:H4'    | 48:BP:7:ARG:HD2     | 1.51                     | 0.90              |
| 35:BA:614(A):U:H4'  | 35:BA:614(B):G:H5'' | 1.54                     | 0.90              |
| 35:DA:2723:C:H5''   | 50:DR:2:ARG:HH11    | 1.36                     | 0.90              |
| 35:BA:2444:G:OP2    | 40:BF:68:LYS:HE2    | 1.72                     | 0.89              |
| 52:BT:125:ARG:HH11  | 52:BT:125:ARG:HA    | 1.34                     | 0.89              |
| 11:CK:111:ASP:HA    | 18:CR:84:LYS:HD2    | 1.50                     | 0.89              |
| 22:CW:51:U:H3       | 22:CW:65:G:H1       | 1.16                     | 0.89              |
| 24:CY:670:VAL:HG23  | 24:CY:671:MET:N     | 1.82                     | 0.89              |
| 35:DA:1899:G:N2     | 35:DA:1902:C:N4     | 2.18                     | 0.89              |
| 39:DE:38:THR:HB     | 39:DE:41:LYS:HG2    | 1.54                     | 0.89              |
| 24:AY:84:THR:H      | 24:AY:85:PRO:CD     | 1.84                     | 0.89              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:1899:G:N2    | 35:BA:1902:C:N4    | 2.19                     | 0.89              |
| 1:CA:720:C:H3'     | 1:CA:721:G:H5''    | 1.55                     | 0.89              |
| 54:DV:28:GLU:HB2   | 54:DV:31:ALA:HB2   | 1.53                     | 0.89              |
| 35:BA:358:U:H2'    | 35:BA:359:A:H8     | 1.36                     | 0.89              |
| 37:BC:118:PRO:HA   | 37:BC:121:MET:HG3  | 1.50                     | 0.89              |
| 38:BD:183:ARG:HG2  | 38:BD:183:ARG:HH11 | 1.37                     | 0.89              |
| 3:CC:90:GLU:O      | 3:CC:93:LYS:HB3    | 1.72                     | 0.89              |
| 35:DA:2308:G:N7    | 35:DA:2310:A:H5'   | 1.87                     | 0.89              |
| 20:AT:23:ARG:O     | 20:AT:27:LYS:HB2   | 1.70                     | 0.89              |
| 18:CR:29:PHE:H     | 18:CR:29:PHE:HD2   | 1.18                     | 0.89              |
| 20:CT:13:LEU:H     | 20:CT:13:LEU:HD12  | 1.36                     | 0.89              |
| 13:AM:96:LEU:HB3   | 13:AM:97:PRO:HD2   | 1.52                     | 0.89              |
| 35:BA:1348:G:H2'   | 35:BA:1349:A:H5''  | 1.52                     | 0.89              |
| 35:BA:192:C:H2'    | 35:BA:193:U:H5'    | 1.55                     | 0.89              |
| 35:BA:813:U:H2'    | 35:BA:814:C:C6     | 2.07                     | 0.89              |
| 54:BV:28:GLU:HB2   | 54:BV:31:ALA:HB2   | 1.54                     | 0.89              |
| 33:D8:33:ASN:H     | 33:D8:33:ASN:ND2   | 1.60                     | 0.89              |
| 39:DE:111:ARG:HA   | 50:DR:2:ARG:HB3    | 1.52                     | 0.89              |
| 4:AD:129:ASN:ND2   | 4:AD:145:GLU:H     | 1.70                     | 0.89              |
| 54:BV:18:LEU:HD22  | 54:BV:19:LYS:H     | 1.38                     | 0.89              |
| 55:DW:5:ALA:HB2    | 55:DW:54:ALA:HB2   | 1.54                     | 0.89              |
| 2:AB:204:ASN:ND2   | 2:AB:206:ASP:H     | 1.71                     | 0.89              |
| 3:AC:50:ALA:HB1    | 3:AC:70:VAL:HG11   | 1.54                     | 0.89              |
| 35:BA:2308:G:N7    | 35:BA:2310:A:H5'   | 1.88                     | 0.89              |
| 3:AC:16:ARG:NH1    | 3:AC:16:ARG:HB2    | 1.87                     | 0.89              |
| 5:AE:50:GLU:HG3    | 5:AE:52:PRO:HD2    | 1.52                     | 0.89              |
| 24:AY:355:LEU:HD12 | 24:AY:369:LEU:HD13 | 1.52                     | 0.89              |
| 37:BC:118:PRO:CA   | 37:BC:121:MET:HG2  | 2.03                     | 0.89              |
| 52:DT:125:ARG:HA   | 52:DT:125:ARG:HH11 | 1.37                     | 0.89              |
| 1:AA:1356:G:H2'    | 1:AA:1357:A:C8     | 2.08                     | 0.89              |
| 22:AV:20:U:H3'     | 22:AV:21:A:H5'     | 1.55                     | 0.89              |
| 28:B3:8:LEU:HD22   | 28:B3:31:LEU:HD23  | 1.53                     | 0.89              |
| 35:BA:1876:A:H2'   | 35:BA:1877:A:H8    | 1.36                     | 0.89              |
| 35:BA:2110:G:O2'   | 35:BA:2120:G:H5'   | 1.71                     | 0.89              |
| 52:BT:85:LYS:NZ    | 52:BT:85:LYS:HB3   | 1.87                     | 0.89              |
| 2:CB:223:ILE:HG12  | 2:CB:226:ARG:NH2   | 1.88                     | 0.89              |
| 27:D2:4:SER:HA     | 27:D2:7:ARG:HH12   | 1.35                     | 0.89              |
| 35:DA:1876:A:H2'   | 35:DA:1877:A:H8    | 1.36                     | 0.89              |
| 35:DA:2523:G:C2'   | 35:DA:2524:G:H5''  | 2.03                     | 0.89              |
| 41:DG:138:GLN:OE1  | 41:DG:153:ARG:HG2  | 1.72                     | 0.89              |
| 2:AB:223:ILE:HG12  | 2:AB:226:ARG:NH2   | 1.88                     | 0.88              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:BF:170:LEU:HB2 | 40:BF:173:VAL:HB   | 1.53                     | 0.88              |
| 50:BR:45:ARG:HG3  | 50:BR:46:GLY:H     | 1.36                     | 0.88              |
| 10:CJ:50:ILE:HD13 | 10:CJ:50:ILE:H     | 1.34                     | 0.88              |
| 10:CJ:55:LYS:CE   | 10:CJ:55:LYS:H     | 1.85                     | 0.88              |
| 24:CY:201:ILE:H   | 24:CY:201:ILE:HD12 | 1.37                     | 0.88              |
| 54:DV:62:LEU:HD21 | 54:DV:95:LEU:HB2   | 1.55                     | 0.88              |
| 49:DQ:56:ARG:HH21 | 58:DZ:180:VAL:HG21 | 1.37                     | 0.88              |
| 4:AD:129:ASN:HD21 | 4:AD:145:GLU:H     | 1.16                     | 0.88              |
| 35:BA:2189:U:H2'  | 35:BA:2190:G:H5''  | 1.55                     | 0.88              |
| 42:BH:157:TYR:CD1 | 42:BH:171:LEU:HD22 | 2.08                     | 0.88              |
| 47:BO:69:ILE:HD13 | 47:BO:77:ILE:HG23  | 1.52                     | 0.88              |
| 51:BS:24:LEU:HB3  | 51:BS:85:VAL:HG12  | 1.52                     | 0.88              |
| 58:BZ:23:LYS:HD3  | 58:BZ:38:TYR:HE1   | 1.36                     | 0.88              |
| 5:CE:9:LYS:HB2    | 5:CE:112:LEU:HD11  | 1.55                     | 0.88              |
| 2:AB:42:ILE:HD11  | 2:AB:202:PRO:HB2   | 1.54                     | 0.88              |
| 35:BA:2317:C:H2'  | 35:BA:2318:G:H5'   | 1.54                     | 0.88              |
| 35:BA:2796:U:H3'  | 35:BA:2799:C:H5'   | 1.55                     | 0.88              |
| 22:CV:49:G:H1     | 22:CV:65:C:H42     | 1.18                     | 0.88              |
| 46:DN:45:ASN:HD22 | 46:DN:45:ASN:H     | 1.15                     | 0.88              |
| 1:AA:939:G:H5''   | 7:AG:102:ARG:NH2   | 1.88                     | 0.88              |
| 35:BA:1658:C:H2'  | 35:BA:1659:U:C6    | 2.08                     | 0.88              |
| 35:BA:1658:C:H2'  | 35:BA:1659:U:H6    | 1.37                     | 0.88              |
| 33:B8:13:ARG:NH1  | 48:BP:59:LEU:HG    | 1.89                     | 0.88              |
| 19:CS:41:VAL:HG21 | 19:CS:44:MET:HB2   | 1.55                     | 0.88              |
| 22:CV:39:C:H2'    | 22:CV:40:C:H6      | 1.39                     | 0.88              |
| 23:CX:13:A:H3'    | 23:CX:14:A:H5''    | 0.92                     | 0.88              |
| 39:DE:33:VAL:HG12 | 39:DE:90:THR:H     | 1.34                     | 0.88              |
| 42:DH:157:TYR:CD1 | 42:DH:171:LEU:HD22 | 2.07                     | 0.88              |
| 1:AA:80:G:H3'     | 1:AA:81:U:C5'      | 2.03                     | 0.88              |
| 2:AB:44:LEU:HD12  | 2:AB:44:LEU:H      | 1.36                     | 0.88              |
| 13:AM:69:GLU:HG2  | 29:B4:43:TYR:OH    | 1.74                     | 0.88              |
| 35:BA:1947:C:C2'  | 35:BA:1948:G:H5''  | 2.04                     | 0.88              |
| 48:BP:85:LEU:HD23 | 48:BP:85:LEU:H     | 1.38                     | 0.88              |
| 35:BA:2723:C:H5'' | 50:BR:2:ARG:HH11   | 1.37                     | 0.88              |
| 2:CB:165:VAL:HG23 | 2:CB:166:ASP:H     | 1.37                     | 0.88              |
| 33:D8:50:LEU:HD12 | 33:D8:51:ALA:H     | 1.39                     | 0.88              |
| 35:DA:2245:U:H5'  | 35:DA:2246:G:H5'   | 1.53                     | 0.88              |
| 56:DX:24:GLY:O    | 56:DX:82:GLN:HA    | 1.72                     | 0.88              |
| 22:AW:31:G:H2'    | 22:AW:32:G:H8      | 1.36                     | 0.88              |
| 31:B6:10:LEU:CD2  | 31:B6:10:LEU:H     | 1.86                     | 0.88              |
| 1:CA:1323:G:H2'   | 1:CA:1324:A:C8     | 2.09                     | 0.88              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:B2:3:LEU:HD22  | 27:B2:7:ARG:NH1    | 1.88                     | 0.88              |
| 35:DA:2645:G:H3'  | 35:DA:2646:C:C5'   | 2.03                     | 0.88              |
| 58:DZ:156:LYS:O   | 58:DZ:158:PRO:HD3  | 1.73                     | 0.88              |
| 24:AY:170:ARG:O   | 24:AY:171:GLU:HG2  | 1.74                     | 0.88              |
| 30:B5:34:PRO:O    | 30:B5:35:GLU:HB2   | 1.74                     | 0.88              |
| 35:BA:1070:A:H5'  | 35:BA:1072:C:OP2   | 1.73                     | 0.88              |
| 35:BA:996:A:H4'   | 53:BU:92:ARG:NE    | 1.87                     | 0.88              |
| 41:BG:97:ASP:H    | 41:BG:100:TRP:HD1  | 1.16                     | 0.88              |
| 54:BV:62:LEU:HD21 | 54:BV:95:LEU:HB2   | 1.54                     | 0.88              |
| 13:CM:97:PRO:HA   | 13:CM:110:ARG:HD3  | 1.56                     | 0.88              |
| 27:D2:25:VAL:HG22 | 27:D2:60:LEU:HD13  | 1.55                     | 0.88              |
| 35:DA:2761:G:H2'  | 35:DA:2762:G:H5''  | 1.53                     | 0.88              |
| 41:DG:55:LYS:HD3  | 41:DG:56:ALA:N     | 1.88                     | 0.88              |
| 35:BA:2761:G:H2'  | 35:BA:2762:G:H5''  | 1.54                     | 0.88              |
| 24:AY:662:LYS:NZ  | 42:BH:175:LYS:CE   | 2.36                     | 0.88              |
| 2:CB:172:ILE:H    | 2:CB:172:ILE:HD12  | 1.38                     | 0.88              |
| 1:CA:1221:G:H4'   | 19:CS:77:THR:HG21  | 1.56                     | 0.88              |
| 20:AT:45:GLN:HB2  | 20:AT:91:LEU:HD13  | 1.56                     | 0.88              |
| 35:BA:2742:C:O2'  | 35:BA:2743:C:H5'   | 1.73                     | 0.88              |
| 39:BE:38:THR:HB   | 39:BE:41:LYS:HG2   | 1.56                     | 0.88              |
| 40:BF:181:LEU:HB3 | 40:BF:205:ARG:NH1  | 1.89                     | 0.88              |
| 1:AA:1364:U:O2    | 1:AA:1364:U:H2'    | 1.72                     | 0.87              |
| 24:AY:488:THR:O   | 24:AY:516:PRO:HG3  | 1.74                     | 0.87              |
| 2:CB:42:ILE:HD11  | 2:CB:202:PRO:HB2   | 1.56                     | 0.87              |
| 12:CL:79:GLU:HB2  | 24:CY:442:THR:HG21 | 1.55                     | 0.87              |
| 35:DA:1782:C:H1'  | 35:DA:2609:U:H5'   | 1.57                     | 0.87              |
| 35:DA:2807:G:H3'  | 35:DA:2808:U:H5''  | 1.57                     | 0.87              |
| 36:DB:91:C:OP1    | 49:DQ:16:ARG:HG3   | 1.74                     | 0.87              |
| 24:AY:409:ILE:CD1 | 24:AY:654:GLY:HA2  | 2.04                     | 0.87              |
| 33:B8:52:LYS:N    | 33:B8:53:PRO:HD2   | 1.89                     | 0.87              |
| 48:BP:39:LYS:HE2  | 48:BP:40:SER:H     | 1.40                     | 0.87              |
| 50:BR:84:ALA:HB3  | 50:BR:85:PRO:HD3   | 1.57                     | 0.87              |
| 17:CQ:59:ILE:HG23 | 17:CQ:71:PHE:HB3   | 1.57                     | 0.87              |
| 35:DA:2103:C:H2'  | 35:DA:2104:G:H5''  | 1.56                     | 0.87              |
| 2:AB:223:ILE:HG12 | 2:AB:226:ARG:CZ    | 2.05                     | 0.87              |
| 7:AG:151:TYR:OH   | 11:AK:54:ARG:HD3   | 1.74                     | 0.87              |
| 30:B5:55:ARG:O    | 30:B5:56:LYS:HB2   | 1.73                     | 0.87              |
| 13:CM:96:LEU:HB3  | 13:CM:97:PRO:HD2   | 1.55                     | 0.87              |
| 35:DA:2317:C:C2'  | 35:DA:2318:G:H5'   | 2.03                     | 0.87              |
| 35:DA:545:C:H2'   | 35:DA:547:A:H5''   | 1.56                     | 0.87              |
| 57:DY:10:GLY:HA2  | 57:DY:27:VAL:HG13  | 1.55                     | 0.87              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:DY:79:CYS:SG    | 57:DY:80:GLY:N     | 2.48                     | 0.87              |
| 35:BA:2645:G:H3'   | 35:BA:2646:C:C5'   | 2.03                     | 0.87              |
| 5:CE:80:ILE:HG22   | 8:CH:104:ARG:NH2   | 1.89                     | 0.87              |
| 52:DT:85:LYS:NZ    | 52:DT:85:LYS:HB3   | 1.89                     | 0.87              |
| 35:BA:1876:A:H2'   | 35:BA:1877:A:C8    | 2.10                     | 0.87              |
| 35:BA:2103:C:H2'   | 35:BA:2104:G:H5''  | 1.56                     | 0.87              |
| 41:BG:76:SER:CB    | 41:BG:83:ARG:HB3   | 2.04                     | 0.87              |
| 57:BY:10:GLY:HA2   | 57:BY:27:VAL:HG13  | 1.56                     | 0.87              |
| 35:DA:1876:A:H2'   | 35:DA:1877:A:C8    | 2.10                     | 0.87              |
| 35:DA:925:C:C2'    | 35:DA:926:A:H5''   | 2.05                     | 0.87              |
| 17:AQ:59:ILE:HG23  | 17:AQ:71:PHE:HB3   | 1.56                     | 0.87              |
| 35:BA:195:A:OP1    | 48:BP:46:LYS:HE2   | 1.73                     | 0.87              |
| 58:DZ:18:LEU:HD12  | 58:DZ:18:LEU:H     | 1.39                     | 0.87              |
| 17:AQ:3:LYS:HB3    | 17:AQ:61:GLU:HB3   | 1.55                     | 0.87              |
| 35:BA:1452:A:C3'   | 35:BA:1453:U:H5''  | 2.03                     | 0.87              |
| 38:DD:158:ALA:HB3  | 38:DD:161:THR:HG21 | 1.56                     | 0.87              |
| 41:DG:51:ARG:HE    | 41:DG:51:ARG:HA    | 1.38                     | 0.87              |
| 48:DP:55:ARG:HG2   | 48:DP:56:SER:N     | 1.83                     | 0.87              |
| 50:DR:84:ALA:HB3   | 50:DR:85:PRO:HD3   | 1.57                     | 0.87              |
| 11:AK:124:LYS:HD2  | 11:AK:125:PHE:HE1  | 1.39                     | 0.87              |
| 17:AQ:52:LYS:HD2   | 17:AQ:52:LYS:H     | 1.40                     | 0.87              |
| 33:B8:56:GLU:HA    | 33:B8:59:LYS:HZ1   | 1.38                     | 0.87              |
| 3:CC:20:SER:HB3    | 3:CC:40:ARG:HH22   | 1.37                     | 0.87              |
| 33:D8:52:LYS:N     | 33:D8:53:PRO:HD2   | 1.90                     | 0.87              |
| 6:AF:67:MET:HB2    | 6:AF:68:PRO:HD2    | 1.57                     | 0.87              |
| 30:B5:2:ALA:CA     | 35:BA:2015:A:H1'   | 2.05                     | 0.87              |
| 35:BA:545:C:H2'    | 35:BA:547:A:H5''   | 1.55                     | 0.87              |
| 52:BT:23:ARG:O     | 52:BT:25:GLY:N     | 2.08                     | 0.87              |
| 3:CC:50:ALA:HB1    | 3:CC:70:VAL:HG11   | 1.54                     | 0.87              |
| 17:CQ:69:LYS:O     | 17:CQ:70:ARG:HD2   | 1.74                     | 0.87              |
| 31:D6:28:ARG:NH1   | 31:D6:28:ARG:HB3   | 1.90                     | 0.87              |
| 35:DA:2175:C:H4'   | 37:DC:219:MET:O    | 1.75                     | 0.87              |
| 1:AA:1251:A:H2'    | 1:AA:1252:A:C8     | 2.09                     | 0.86              |
| 1:AA:1323:G:H2'    | 1:AA:1324:A:C8     | 2.11                     | 0.86              |
| 44:BK:30:HIS:HA    | 44:BK:59:ILE:HD12  | 1.56                     | 0.86              |
| 1:CA:656:C:H4'     | 15:CO:62:GLN:NE2   | 1.88                     | 0.86              |
| 11:CK:124:LYS:HD2  | 11:CK:125:PHE:HE1  | 1.38                     | 0.86              |
| 24:CY:272:LEU:O    | 24:CY:276:VAL:HG23 | 1.75                     | 0.86              |
| 24:CY:605:ILE:HD11 | 24:CY:677:GLN:HG2  | 1.57                     | 0.86              |
| 25:D0:60:PHE:CE2   | 35:DA:2365:G:H4'   | 2.09                     | 0.86              |
| 35:DA:2425:A:H5'   | 35:DA:2427:C:O4'   | 1.75                     | 0.86              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 6:AF:43:LEU:H      | 6:AF:43:LEU:HD12    | 1.40                     | 0.86              |
| 10:AJ:37:PRO:HA    | 10:AJ:72:VAL:HG22   | 1.56                     | 0.86              |
| 24:AY:468:ARG:HB3  | 24:AY:468:ARG:HH11  | 1.39                     | 0.86              |
| 1:CA:1502:A:H2     | 1:CA:1505:G:H1      | 1.23                     | 0.86              |
| 1:CA:80:G:H3'      | 1:CA:81:U:C5'       | 2.04                     | 0.86              |
| 20:CT:45:GLN:HB2   | 20:CT:91:LEU:HD13   | 1.55                     | 0.86              |
| 25:B0:60:PHE:CE2   | 35:BA:2365:G:H4'    | 2.10                     | 0.86              |
| 35:BA:1658:C:OP1   | 39:BE:132:HIS:ND1   | 2.08                     | 0.86              |
| 6:CF:67:MET:HB2    | 6:CF:68:PRO:HD2     | 1.58                     | 0.86              |
| 35:DA:614(A):U:H4' | 35:DA:614(B):G:H5'' | 1.56                     | 0.86              |
| 48:DP:85:LEU:HD23  | 48:DP:85:LEU:H      | 1.39                     | 0.86              |
| 35:BA:108:U:H2'    | 35:BA:109:G:C8      | 2.10                     | 0.86              |
| 49:BQ:45:GLN:H     | 49:BQ:45:GLN:NE2    | 1.74                     | 0.86              |
| 1:CA:483:C:H3'     | 1:CA:484:G:H5''     | 1.55                     | 0.86              |
| 3:CC:70:VAL:HG12   | 3:CC:71:ALA:N       | 1.90                     | 0.86              |
| 28:D3:17:LYS:NZ    | 28:D3:20:LYS:HE3    | 1.91                     | 0.86              |
| 33:D8:13:ARG:NH1   | 48:DP:59:LEU:HG     | 1.90                     | 0.86              |
| 3:AC:20:SER:HB3    | 3:AC:40:ARG:NH2     | 1.91                     | 0.86              |
| 1:AA:973:G:O4'     | 10:AJ:55:LYS:HG3    | 1.75                     | 0.86              |
| 35:BA:1223:G:H3'   | 35:BA:1224:C:H5''   | 1.58                     | 0.86              |
| 35:BA:2562:U:H1'   | 47:BO:23:ARG:HH11   | 1.39                     | 0.86              |
| 49:BQ:59:ARG:HA    | 58:BZ:180:VAL:HG23  | 1.58                     | 0.86              |
| 3:CC:16:ARG:NH1    | 3:CC:16:ARG:HB2     | 1.91                     | 0.86              |
| 35:DA:1285:G:H2'   | 35:DA:1286:A:H5'    | 1.57                     | 0.86              |
| 50:DR:38:VAL:HB    | 50:DR:39:PRO:HD3    | 1.56                     | 0.86              |
| 5:AE:9:LYS:HB2     | 5:AE:112:LEU:HD11   | 1.57                     | 0.86              |
| 12:AL:41:ARG:HH11  | 12:AL:41:ARG:HB3    | 1.41                     | 0.86              |
| 1:AA:656:C:H4'     | 15:AO:62:GLN:NE2    | 1.89                     | 0.86              |
| 35:BA:1899:G:H22   | 35:BA:1902:C:H41    | 1.21                     | 0.86              |
| 35:DA:192:C:H2'    | 35:DA:193:U:H5'     | 1.57                     | 0.86              |
| 37:DC:77:ALA:HB3   | 37:DC:95:VAL:HA     | 1.57                     | 0.86              |
| 48:DP:40:SER:O     | 48:DP:41:ARG:HD2    | 1.76                     | 0.86              |
| 39:BE:24:THR:HG22  | 39:BE:186:GLY:HA2   | 1.58                     | 0.86              |
| 5:CE:102:ALA:HB2   | 5:CE:120:THR:OG1    | 1.76                     | 0.86              |
| 10:CJ:6:ILE:HD11   | 10:CJ:72:VAL:CB     | 2.04                     | 0.86              |
| 17:CQ:52:LYS:H     | 17:CQ:52:LYS:HD2    | 1.40                     | 0.86              |
| 18:CR:56:THR:HB    | 18:CR:58:LEU:HD13   | 1.57                     | 0.86              |
| 35:DA:2562:U:H1'   | 47:DO:23:ARG:HH11   | 1.41                     | 0.86              |
| 36:DB:65:C:N4      | 36:DB:109:C:H2'     | 1.91                     | 0.86              |
| 40:DF:24:LEU:HB3   | 40:DF:25:PRO:HD2    | 1.56                     | 0.86              |
| 1:AA:697:U:H2'     | 1:AA:698:G:H5'      | 1.57                     | 0.86              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:BT:13:ARG:HA    | 52:BT:13:ARG:CZ    | 2.06                     | 0.86              |
| 1:CA:697:U:H2'     | 1:CA:698:G:H5'     | 1.58                     | 0.86              |
| 35:DA:27:G:N2      | 35:DA:512:G:H2'    | 1.90                     | 0.86              |
| 39:DE:176:ILE:HG22 | 39:DE:178:GLU:HB3  | 1.55                     | 0.86              |
| 57:DY:44:ILE:HG22  | 57:DY:45:VAL:H     | 1.41                     | 0.86              |
| 35:BA:203:C:H3'    | 35:BA:204:A:H5''   | 1.58                     | 0.86              |
| 35:BA:2317:C:C2'   | 35:BA:2318:G:H5'   | 2.05                     | 0.86              |
| 35:BA:2876:G:H4'   | 52:BT:3:ARG:HE     | 1.41                     | 0.86              |
| 2:CB:223:ILE:HG12  | 2:CB:226:ARG:CZ    | 2.05                     | 0.86              |
| 17:CQ:3:LYS:HB3    | 17:CQ:61:GLU:HB3   | 1.56                     | 0.86              |
| 35:DA:2796:U:H3'   | 35:DA:2799:C:H5'   | 1.55                     | 0.86              |
| 35:DA:940:G:H5'    | 35:DA:941:A:OP2    | 1.75                     | 0.86              |
| 39:DE:60:ASN:OD1   | 39:DE:62:PRO:HD2   | 1.76                     | 0.86              |
| 41:DG:77:ILE:HG21  | 41:DG:80:PHE:HB2   | 1.56                     | 0.86              |
| 57:DY:10:GLY:CA    | 57:DY:27:VAL:HG13  | 2.05                     | 0.86              |
| 15:AO:78:TYR:O     | 15:AO:82:ILE:HG22  | 1.76                     | 0.86              |
| 35:BA:1285:G:H2'   | 35:BA:1286:A:H5'   | 1.58                     | 0.86              |
| 55:BW:5:ALA:HB2    | 55:BW:54:ALA:HB2   | 1.57                     | 0.86              |
| 35:DA:978:G:H1     | 35:DA:985:C:H42    | 1.23                     | 0.86              |
| 35:DA:1818:U:H5''  | 38:DD:157:ARG:HB2  | 1.57                     | 0.86              |
| 40:DF:53:THR:HG23  | 40:DF:55:GLY:N     | 1.91                     | 0.86              |
| 35:BA:27:G:N2      | 35:BA:512:G:H2'    | 1.90                     | 0.85              |
| 38:BD:35:LYS:HZ3   | 38:BD:36:PRO:CD    | 1.89                     | 0.85              |
| 42:BH:17:VAL:HG11  | 42:BH:50:VAL:HG21  | 1.56                     | 0.85              |
| 57:BY:10:GLY:CA    | 57:BY:27:VAL:HG13  | 2.06                     | 0.85              |
| 2:CB:29:ALA:O      | 2:CB:32:ILE:HG22   | 1.76                     | 0.85              |
| 12:CL:41:ARG:HH11  | 12:CL:41:ARG:HB3   | 1.38                     | 0.85              |
| 30:D5:2:ALA:CA     | 35:DA:2015:A:H1'   | 2.04                     | 0.85              |
| 40:DF:181:LEU:HB3  | 40:DF:205:ARG:NH1  | 1.91                     | 0.85              |
| 36:DB:103:G:H21    | 58:DZ:73:GLN:HE22  | 1.23                     | 0.85              |
| 26:B1:41:ARG:NH2   | 35:BA:1365:A:H5'   | 1.91                     | 0.85              |
| 42:BH:169:VAL:HG22 | 42:BH:170:ARG:H    | 1.40                     | 0.85              |
| 52:BT:46:GLU:O     | 52:BT:65:LYS:HD2   | 1.75                     | 0.85              |
| 49:BQ:56:ARG:HH21  | 58:BZ:180:VAL:HG21 | 1.40                     | 0.85              |
| 1:CA:579:G:H5'     | 1:CA:728:A:H1'     | 1.57                     | 0.85              |
| 24:CY:519:ARG:NH1  | 24:CY:678:GLU:H    | 1.74                     | 0.85              |
| 35:DA:1658:C:H2'   | 35:DA:1659:U:C6    | 2.12                     | 0.85              |
| 35:DA:2742:C:O2'   | 35:DA:2743:C:H5'   | 1.76                     | 0.85              |
| 41:DG:112:PRO:O    | 41:DG:113:ARG:HA   | 1.76                     | 0.85              |
| 42:DH:17:VAL:HG11  | 42:DH:50:VAL:HG21  | 1.57                     | 0.85              |
| 52:DT:29:ARG:CB    | 52:DT:85:LYS:HA    | 2.05                     | 0.85              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:AA:1004:A:H61     | 1:AA:1034:G:H2'    | 1.40                     | 0.85              |
| 27:D2:69:ARG:HG3    | 27:D2:70:GLN:N     | 1.91                     | 0.85              |
| 30:D5:4:HIS:HB3     | 30:D5:5:PRO:HD3    | 1.56                     | 0.85              |
| 49:DQ:45:GLN:NE2    | 49:DQ:45:GLN:H     | 1.73                     | 0.85              |
| 2:AB:22:LYS:HE2     | 2:AB:22:LYS:HA     | 1.57                     | 0.85              |
| 10:AJ:55:LYS:H      | 10:AJ:55:LYS:HE2   | 1.41                     | 0.85              |
| 26:B1:45:ASN:HD21   | 26:B1:47:GLN:HE21  | 1.24                     | 0.85              |
| 37:BC:77:ALA:HB3    | 37:BC:95:VAL:HA    | 1.58                     | 0.85              |
| 40:BF:24:LEU:HB3    | 40:BF:25:PRO:HD2   | 1.57                     | 0.85              |
| 1:CA:1004:A:H61     | 1:CA:1034:G:H2'    | 1.40                     | 0.85              |
| 30:D5:55:ARG:O      | 30:D5:56:LYS:HB2   | 1.74                     | 0.85              |
| 40:DF:84:VAL:HG12   | 40:DF:85:GLY:H     | 1.39                     | 0.85              |
| 33:B8:50:LEU:HD12   | 33:B8:51:ALA:H     | 1.38                     | 0.85              |
| 39:BE:60:ASN:OD1    | 39:BE:62:PRO:HD2   | 1.74                     | 0.85              |
| 42:BH:12:PRO:HB2    | 42:BH:15:VAL:HG11  | 1.57                     | 0.85              |
| 35:DA:1826:G:H4'    | 38:DD:242:ARG:HH21 | 1.40                     | 0.85              |
| 57:DY:94:LYS:C      | 57:DY:102:CYS:HB2  | 1.97                     | 0.85              |
| 35:BA:1747(A):G:H2' | 35:BA:1748:G:C5'   | 2.07                     | 0.85              |
| 1:CA:148:G:H2'      | 1:CA:149:A:H8      | 1.41                     | 0.85              |
| 4:CD:30:LYS:C       | 4:CD:32:ALA:H      | 1.80                     | 0.85              |
| 8:CH:83:ILE:HD12    | 8:CH:137:VAL:HG22  | 1.58                     | 0.85              |
| 29:D4:14:ILE:O      | 29:D4:21:VAL:HG13  | 1.77                     | 0.85              |
| 42:DH:169:VAL:HG22  | 42:DH:170:ARG:H    | 1.39                     | 0.85              |
| 52:DT:46:GLU:O      | 52:DT:65:LYS:HD2   | 1.76                     | 0.85              |
| 58:DZ:130:PRO:HA    | 58:DZ:133:ILE:HD11 | 1.58                     | 0.85              |
| 40:BF:53:THR:HG23   | 40:BF:55:GLY:N     | 1.90                     | 0.85              |
| 50:BR:100:LEU:HD22  | 50:BR:100:LEU:H    | 1.39                     | 0.85              |
| 1:CA:1057:G:H5''    | 3:CC:154:SER:CB    | 2.06                     | 0.85              |
| 35:DA:2524:G:H8     | 35:DA:2524:G:H5'   | 1.41                     | 0.85              |
| 35:DA:272(H):C:H5'  | 35:DA:272(H):C:H6  | 1.41                     | 0.85              |
| 44:DK:30:HIS:HA     | 44:DK:59:ILE:HD12  | 1.56                     | 0.85              |
| 46:DN:91:LEU:HD23   | 46:DN:98:VAL:HG21  | 1.57                     | 0.85              |
| 35:DA:2876:G:H4'    | 52:DT:3:ARG:HE     | 1.41                     | 0.85              |
| 10:AJ:75:ILE:HG13   | 10:AJ:76:ASN:N     | 1.92                     | 0.85              |
| 24:AY:416:LYS:CD    | 24:AY:417:THR:H    | 1.89                     | 0.85              |
| 24:AY:517:LEU:HD23  | 24:AY:521:SER:HB3  | 1.57                     | 0.85              |
| 35:BA:1782:C:H1'    | 35:BA:2609:U:H5'   | 1.56                     | 0.85              |
| 35:BA:1818:U:H5''   | 38:BD:157:ARG:HB2  | 1.58                     | 0.85              |
| 50:BR:73:VAL:O      | 50:BR:76:VAL:HG12  | 1.77                     | 0.85              |
| 5:CE:64:ARG:HH11    | 5:CE:64:ARG:HG3    | 1.42                     | 0.85              |
| 26:D1:73:LEU:HD21   | 26:D1:94:LEU:HB3   | 1.57                     | 0.85              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:2317:C:H2'   | 35:DA:2318:G:H5'   | 1.55                     | 0.85              |
| 41:DG:35:GLU:HB3   | 41:DG:160:VAL:HG12 | 1.59                     | 0.85              |
| 42:DH:12:PRO:HB2   | 42:DH:15:VAL:HG11  | 1.56                     | 0.85              |
| 50:DR:117:VAL:O    | 50:DR:118:GLU:HB2  | 1.77                     | 0.85              |
| 58:DZ:48:PHE:CE1   | 58:DZ:52:SER:HA    | 2.12                     | 0.85              |
| 31:B6:28:ARG:NH1   | 31:B6:28:ARG:HB3   | 1.91                     | 0.85              |
| 35:BA:940:G:H5'    | 35:BA:941:A:OP2    | 1.76                     | 0.85              |
| 36:BB:3:C:H42      | 36:BB:118:G:H1     | 1.25                     | 0.85              |
| 42:BH:30:LYS:HD2   | 42:BH:81:GLU:HG2   | 1.59                     | 0.85              |
| 51:BS:106:ARG:HB3  | 51:BS:106:ARG:HH11 | 1.42                     | 0.85              |
| 52:BT:29:ARG:CB    | 52:BT:85:LYS:HA    | 2.06                     | 0.85              |
| 2:CB:22:LYS:HE2    | 2:CB:22:LYS:HA     | 1.59                     | 0.85              |
| 35:DA:1779:U:H5    | 35:DA:1784:A:N7    | 1.74                     | 0.85              |
| 2:AB:172:ILE:HD12  | 2:AB:172:ILE:H     | 1.40                     | 0.85              |
| 13:AM:97:PRO:HA    | 13:AM:110:ARG:HD3  | 1.56                     | 0.85              |
| 29:B4:10:VAL:HG23  | 29:B4:11:PRO:HD2   | 1.58                     | 0.85              |
| 41:BG:97:ASP:HB2   | 41:BG:98:ARG:HH12  | 1.42                     | 0.85              |
| 1:CA:1495:U:H2'    | 1:CA:1496:C:H6     | 1.42                     | 0.85              |
| 24:CY:489:LYS:HG2  | 24:CY:598:ASP:HB2  | 1.58                     | 0.85              |
| 35:DA:2502:G:H5''  | 35:DA:2503:A:H5'   | 1.59                     | 0.85              |
| 51:DS:106:ARG:HB3  | 51:DS:106:ARG:HH11 | 1.41                     | 0.85              |
| 52:DT:53:ARG:HB3   | 52:DT:53:ARG:NH1   | 1.92                     | 0.85              |
| 58:DZ:137:ILE:HG21 | 58:DZ:155:LEU:HD12 | 1.57                     | 0.85              |
| 1:AA:579:G:H5'     | 1:AA:728:A:H1'     | 1.58                     | 0.84              |
| 9:AI:95:LYS:HZ3    | 9:AI:96:LEU:HD12   | 1.41                     | 0.84              |
| 35:BA:1826:G:H4'   | 38:BD:242:ARG:HH21 | 1.42                     | 0.84              |
| 10:CJ:75:ILE:HG13  | 10:CJ:76:ASN:N     | 1.89                     | 0.84              |
| 24:CY:148:LEU:HA   | 24:CY:151:ARG:HD2  | 1.57                     | 0.84              |
| 35:DA:1609:A:H5'   | 35:DA:1610:A:OP2   | 1.75                     | 0.84              |
| 35:DA:1678:G:N2    | 35:DA:1989:G:H22   | 1.74                     | 0.84              |
| 35:DA:2444:G:OP2   | 40:DF:68:LYS:HE2   | 1.76                     | 0.84              |
| 36:DB:3:C:H42      | 36:DB:118:G:H1     | 1.25                     | 0.84              |
| 43:DJ:26:UNK:HA    | 43:DJ:84:UNK:HA    | 1.60                     | 0.84              |
| 35:BA:107:C:H2'    | 35:BA:108:U:H6     | 1.41                     | 0.84              |
| 35:BA:2502:G:H5''  | 35:BA:2503:A:H5'   | 1.59                     | 0.84              |
| 35:BA:2645:G:H4'   | 35:BA:2732:G:O2'   | 1.77                     | 0.84              |
| 35:BA:2807:G:H3'   | 35:BA:2808:U:H5''  | 1.57                     | 0.84              |
| 36:BB:87:G:H2'     | 36:BB:88:C:H3'     | 1.58                     | 0.84              |
| 52:BT:53:ARG:NH1   | 52:BT:53:ARG:HB3   | 1.91                     | 0.84              |
| 25:D0:40:GLN:NE2   | 25:D0:43:THR:HA    | 1.92                     | 0.84              |
| 35:DA:1242:A:H5'   | 35:DA:1243:G:OP2   | 1.77                     | 0.84              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:DD:183:ARG:HG2  | 38:DD:183:ARG:HH11 | 1.41                     | 0.84              |
| 41:DG:87:PRO:O     | 41:DG:88:ILE:HD12  | 1.77                     | 0.84              |
| 52:DT:132:LYS:H    | 52:DT:132:LYS:HD3  | 1.42                     | 0.84              |
| 25:B0:50:ASN:HA    | 25:B0:62:LEU:HD12  | 1.59                     | 0.84              |
| 35:BA:2394:C:OP1   | 48:BP:63:PRO:HD2   | 1.77                     | 0.84              |
| 51:BS:101:LEU:O    | 51:BS:101:LEU:HD12 | 1.77                     | 0.84              |
| 1:CA:973:G:O4'     | 10:CJ:55:LYS:HG3   | 1.77                     | 0.84              |
| 36:DB:87:G:H2'     | 36:DB:88:C:H3'     | 1.59                     | 0.84              |
| 35:DA:1658:C:OP1   | 39:DE:132:HIS:ND1  | 2.09                     | 0.84              |
| 35:BA:1242:A:H5'   | 35:BA:1243:G:OP2   | 1.76                     | 0.84              |
| 35:BA:666:G:H4'    | 48:BP:49:ARG:NH2   | 1.92                     | 0.84              |
| 35:BA:925:C:C2'    | 35:BA:926:A:H5''   | 2.06                     | 0.84              |
| 35:BA:970:C:H2'    | 35:BA:971:C:H6     | 1.42                     | 0.84              |
| 42:BH:118:PRO:HG2  | 42:BH:121:ILE:HD12 | 1.60                     | 0.84              |
| 9:CI:88:TYR:O      | 9:CI:89:ASN:HB2    | 1.77                     | 0.84              |
| 24:CY:170:ARG:HD2  | 24:CY:170:ARG:H    | 1.41                     | 0.84              |
| 24:CY:201:ILE:HG21 | 24:CY:206:LEU:HA   | 1.60                     | 0.84              |
| 38:DD:131:LEU:N    | 38:DD:131:LEU:HD12 | 1.93                     | 0.84              |
| 52:DT:13:ARG:CZ    | 52:DT:13:ARG:HA    | 2.07                     | 0.84              |
| 38:BD:95:LEU:HD12  | 38:BD:103:ARG:O    | 1.78                     | 0.84              |
| 1:CA:299:G:H2'     | 1:CA:300:A:C8      | 2.12                     | 0.84              |
| 13:CM:68:GLY:H     | 13:CM:71:ARG:HB3   | 1.41                     | 0.84              |
| 50:DR:10:LEU:HB3   | 50:DR:17:ARG:HD3   | 1.58                     | 0.84              |
| 24:AY:555:LEU:HD21 | 24:AY:599:PRO:HG3  | 1.60                     | 0.84              |
| 35:BA:2175:C:H4'   | 37:BC:219:MET:O    | 1.76                     | 0.84              |
| 46:BN:91:LEU:HD23  | 46:BN:98:VAL:HG21  | 1.59                     | 0.84              |
| 48:BP:27:HIS:HD2   | 48:BP:28:GLY:N     | 1.74                     | 0.84              |
| 3:CC:83:ARG:O      | 3:CC:86:VAL:HG22   | 1.78                     | 0.84              |
| 35:DA:108:U:H2'    | 35:DA:109:G:C8     | 2.12                     | 0.84              |
| 4:AD:49:ARG:HE     | 4:AD:49:ARG:HA     | 1.43                     | 0.84              |
| 58:BZ:115:GLY:H    | 58:BZ:177:PRO:HG3  | 1.43                     | 0.84              |
| 9:CI:114:TYR:HE1   | 10:CJ:60:ARG:H     | 1.22                     | 0.84              |
| 24:CY:17:ILE:H     | 24:CY:17:ILE:HD12  | 1.41                     | 0.84              |
| 35:DA:978:G:H1     | 35:DA:985:C:N4     | 1.76                     | 0.84              |
| 41:DG:145:THR:HG23 | 41:DG:148:MET:HB2  | 1.59                     | 0.84              |
| 41:DG:145:THR:CG2  | 41:DG:148:MET:HB2  | 2.08                     | 0.84              |
| 46:DN:62:VAL:HG22  | 46:DN:66:LYS:HG3   | 1.59                     | 0.84              |
| 58:DZ:10:ARG:HH21  | 58:DZ:26:GLY:H     | 1.22                     | 0.84              |
| 1:AA:148:G:H2'     | 1:AA:149:A:H8      | 1.42                     | 0.84              |
| 13:AM:68:GLY:H     | 13:AM:71:ARG:HB3   | 1.42                     | 0.84              |
| 18:AR:56:THR:HB    | 18:AR:58:LEU:HD13  | 1.59                     | 0.84              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 35:BA:1947:C:H2'    | 35:BA:1948:G:H5''  | 1.58                     | 0.84              |
| 38:BD:158:ALA:HB3   | 38:BD:161:THR:HG21 | 1.59                     | 0.84              |
| 39:BE:176:ILE:HG22  | 39:BE:178:GLU:HB3  | 1.57                     | 0.84              |
| 52:BT:108:ARG:HG3   | 52:BT:109:GLU:N    | 1.93                     | 0.84              |
| 57:BY:94:LYS:C      | 57:BY:102:CYS:HB2  | 1.98                     | 0.84              |
| 15:CO:78:TYR:O      | 15:CO:82:ILE:HG22  | 1.78                     | 0.84              |
| 22:CW:74:A:H2'      | 22:CW:75:C:H5''    | 1.59                     | 0.84              |
| 24:CY:670:VAL:CG2   | 24:CY:671:MET:H    | 1.89                     | 0.84              |
| 31:D6:10:LEU:H      | 31:D6:10:LEU:CD2   | 1.90                     | 0.84              |
| 35:BA:2425:A:H5'    | 35:BA:2427:C:O4'   | 1.78                     | 0.84              |
| 39:BE:24:THR:HG23   | 39:BE:184:VAL:HG23 | 1.58                     | 0.84              |
| 24:CY:13:ARG:HB3    | 24:CY:79:ILE:HG23  | 1.59                     | 0.84              |
| 35:DA:666:G:H4'     | 48:DP:49:ARG:NH2   | 1.93                     | 0.84              |
| 38:DD:145:VAL:HG22  | 38:DD:191:ALA:HB1  | 1.59                     | 0.84              |
| 44:DK:77:LEU:HD23   | 44:DK:77:LEU:H     | 1.43                     | 0.84              |
| 1:AA:1057:G:H5''    | 3:AC:154:SER:CB    | 2.08                     | 0.84              |
| 35:BA:978:G:H1      | 35:BA:985:C:N4     | 1.75                     | 0.84              |
| 4:CD:194:LEU:HB3    | 4:CD:196:LEU:HD13  | 1.57                     | 0.84              |
| 35:DA:107:C:H2'     | 35:DA:108:U:H6     | 1.41                     | 0.84              |
| 35:DA:2438:U:O3'    | 35:DA:2439:A:H4'   | 1.78                     | 0.84              |
| 42:DH:118:PRO:HG2   | 42:DH:121:ILE:HD12 | 1.60                     | 0.84              |
| 24:AY:329:ARG:HD3   | 24:AY:374:LEU:HD11 | 1.59                     | 0.83              |
| 36:BB:65:C:N4       | 36:BB:109:C:H2'    | 1.91                     | 0.83              |
| 1:CA:814:A:H2'      | 1:CA:816:A:H5'     | 1.60                     | 0.83              |
| 10:CJ:55:LYS:H      | 10:CJ:55:LYS:HE2   | 1.42                     | 0.83              |
| 50:DR:99:LYS:H      | 50:DR:99:LYS:CD    | 1.87                     | 0.83              |
| 58:DZ:81:ARG:NH1    | 58:DZ:81:ARG:HB3   | 1.91                     | 0.83              |
| 25:D0:47:PRO:HG3    | 25:D0:59:LEU:HD21  | 1.58                     | 0.83              |
| 28:D3:29:ARG:HB2    | 28:D3:29:ARG:HH11  | 1.43                     | 0.83              |
| 35:DA:6:A:O2'       | 46:DN:130:HIS:HB2  | 1.77                     | 0.83              |
| 41:DG:68:PRO:HA     | 41:DG:92:VAL:HG13  | 1.57                     | 0.83              |
| 35:DA:1142(A):A:H4' | 46:DN:25:ARG:HH22  | 1.42                     | 0.83              |
| 24:AY:15:ILE:HD11   | 24:AY:81:ILE:HG12  | 1.61                     | 0.83              |
| 46:BN:9:VAL:HG11    | 46:BN:39:ARG:NH2   | 1.92                     | 0.83              |
| 41:DG:76:SER:HB2    | 41:DG:83:ARG:HB3   | 1.58                     | 0.83              |
| 42:BH:16:SER:HB2    | 42:BH:27:LYS:HB2   | 1.60                     | 0.83              |
| 6:CF:43:LEU:H       | 6:CF:43:LEU:HD12   | 1.42                     | 0.83              |
| 10:CJ:7:LYS:HB2     | 10:CJ:97:GLU:HB2   | 1.60                     | 0.83              |
| 40:DF:7:TYR:HD2     | 40:DF:16:GLY:HA3   | 1.43                     | 0.83              |
| 41:DG:86:MET:N      | 41:DG:87:PRO:HD3   | 1.94                     | 0.83              |
| 52:DT:108:ARG:HG3   | 52:DT:109:GLU:N    | 1.92                     | 0.83              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1456:G:H2'    | 1:AA:1457:G:H5'    | 1.60                     | 0.83              |
| 3:AC:70:VAL:HG12   | 3:AC:71:ALA:N      | 1.90                     | 0.83              |
| 11:AK:124:LYS:HD2  | 11:AK:125:PHE:CE1  | 2.14                     | 0.83              |
| 1:AA:368:U:P       | 24:AY:351:ARG:HH11 | 2.01                     | 0.83              |
| 31:B6:51:GLU:O     | 31:B6:52:VAL:HB    | 1.77                     | 0.83              |
| 35:BA:272(H):C:H5' | 35:BA:272(H):C:H6  | 1.41                     | 0.83              |
| 47:BO:43:VAL:HG23  | 47:BO:56:ASP:O     | 1.77                     | 0.83              |
| 1:CA:1438:G:H2'    | 1:CA:1439:C:C6     | 2.14                     | 0.83              |
| 1:CA:980:C:H5      | 1:CA:981:U:C2      | 1.95                     | 0.83              |
| 24:CY:230:LYS:HZ1  | 24:CY:237:PRO:HA   | 1.43                     | 0.83              |
| 24:CY:526:VAL:HB   | 24:CY:566:THR:HA   | 1.60                     | 0.83              |
| 25:D0:14:ARG:NH1   | 25:D0:14:ARG:HB2   | 1.93                     | 0.83              |
| 13:CM:69:GLU:HG2   | 29:D4:43:TYR:OH    | 1.78                     | 0.83              |
| 31:D6:51:GLU:O     | 31:D6:52:VAL:HB    | 1.78                     | 0.83              |
| 35:DA:2287:A:N6    | 35:DA:2344:U:H3    | 1.75                     | 0.83              |
| 38:DD:35:LYS:HZ3   | 38:DD:36:PRO:CD    | 1.92                     | 0.83              |
| 42:DH:16:SER:HB2   | 42:DH:27:LYS:HB2   | 1.59                     | 0.83              |
| 47:DO:24:VAL:HG21  | 47:DO:30:ALA:HB3   | 1.61                     | 0.83              |
| 58:DZ:10:ARG:HH21  | 58:DZ:26:GLY:N     | 1.74                     | 0.83              |
| 1:AA:975:A:H5'     | 1:AA:975:A:H8      | 1.44                     | 0.83              |
| 4:AD:194:LEU:HB3   | 4:AD:196:LEU:HD13  | 1.59                     | 0.83              |
| 16:AP:20:VAL:HG21  | 16:AP:32:TYR:CB    | 2.08                     | 0.83              |
| 35:BA:2287:A:N6    | 35:BA:2344:U:H3    | 1.74                     | 0.83              |
| 35:BA:2438:U:O3'   | 35:BA:2439:A:H4'   | 1.76                     | 0.83              |
| 41:BG:111:LEU:HB2  | 41:BG:112:PRO:HD3  | 1.60                     | 0.83              |
| 41:BG:64:THR:HG23  | 41:BG:66:GLN:H     | 1.44                     | 0.83              |
| 57:BY:44:ILE:HG22  | 57:BY:45:VAL:H     | 1.43                     | 0.83              |
| 61:CY:702:FUA:H122 | 61:CY:702:FUA:H231 | 1.59                     | 0.83              |
| 46:DN:9:VAL:HG11   | 46:DN:39:ARG:NH2   | 1.92                     | 0.83              |
| 47:DO:69:ILE:HD13  | 47:DO:77:ILE:HG23  | 1.59                     | 0.83              |
| 4:AD:30:LYS:C      | 4:AD:32:ALA:H      | 1.79                     | 0.83              |
| 31:B6:48:VAL:HG23  | 31:B6:49:HIS:N     | 1.93                     | 0.83              |
| 35:BA:1678:G:N2    | 35:BA:1989:G:H22   | 1.77                     | 0.83              |
| 40:BF:84:VAL:HG12  | 40:BF:85:GLY:H     | 1.41                     | 0.83              |
| 47:BO:114:ILE:HD12 | 47:BO:114:ILE:H    | 1.43                     | 0.83              |
| 57:BY:46:LYS:H     | 57:BY:62:GLU:HB2   | 1.43                     | 0.83              |
| 10:CJ:49:VAL:HG23  | 14:CN:41:ARG:HB2   | 1.60                     | 0.83              |
| 26:D1:76:ARG:NH1   | 26:D1:95:LEU:HD22  | 1.94                     | 0.83              |
| 30:D5:34:PRO:O     | 30:D5:35:GLU:HB2   | 1.76                     | 0.83              |
| 35:DA:1223:G:H3'   | 35:DA:1224:C:H5''  | 1.57                     | 0.83              |
| 35:DA:1485:G:H1'   | 35:DA:1505:C:H42   | 1.44                     | 0.83              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 35:DA:195:A:OP1     | 48:DP:46:LYS:HE2   | 1.78                     | 0.83              |
| 35:DA:218:A:C2      | 35:DA:235:U:H4'    | 2.13                     | 0.83              |
| 49:DQ:30:GLY:HA2    | 49:DQ:107:ALA:HB2  | 1.60                     | 0.83              |
| 1:AA:980:C:H5       | 1:AA:981:U:C2      | 1.96                     | 0.83              |
| 23:AX:13:A:H3'      | 23:AX:14:A:C5'     | 2.08                     | 0.83              |
| 29:B4:14:ILE:O      | 29:B4:21:VAL:HG13  | 1.77                     | 0.83              |
| 35:BA:806:C:OP2     | 48:BP:39:LYS:HD3   | 1.78                     | 0.83              |
| 35:BA:9:U:H5        | 35:BA:2629:A:H62   | 1.27                     | 0.83              |
| 1:CA:1318:A:H1'     | 19:CS:37:ARG:NH2   | 1.93                     | 0.83              |
| 22:CW:7:G:H3'       | 22:CW:8:U:H5'      | 1.59                     | 0.83              |
| 27:D2:32:LEU:HA     | 27:D2:53:LEU:HD13  | 1.61                     | 0.83              |
| 35:DA:1059:G:H2'    | 35:DA:1060:U:C5    | 2.14                     | 0.83              |
| 48:DP:57:THR:OG1    | 48:DP:59:LEU:HB3   | 1.78                     | 0.83              |
| 1:AA:1221:G:H4'     | 19:AS:77:THR:HG21  | 1.59                     | 0.83              |
| 1:AA:1284:C:H3'     | 1:AA:1285:A:H5''   | 1.61                     | 0.83              |
| 35:BA:1609:A:H5'    | 35:BA:1610:A:OP2   | 1.79                     | 0.83              |
| 40:BF:40:GLN:NE2    | 40:BF:182:ASN:HB2  | 1.93                     | 0.83              |
| 53:BU:31:SER:HB3    | 53:BU:34:LYS:HB2   | 1.61                     | 0.83              |
| 24:CY:21:ILE:HG21   | 24:CY:88:VAL:HG13  | 1.61                     | 0.83              |
| 30:D5:55:ARG:HD3    | 30:D5:55:ARG:C     | 1.98                     | 0.83              |
| 35:DA:2314:C:O2'    | 35:DA:2315:G:H5'   | 1.78                     | 0.83              |
| 48:DP:125:VAL:O     | 48:DP:145:PRO:HD2  | 1.77                     | 0.83              |
| 48:DP:23:PRO:HB2    | 48:DP:33:ARG:HG3   | 1.60                     | 0.83              |
| 1:AA:243:A:H4'      | 1:AA:244:U:O5'     | 1.79                     | 0.83              |
| 10:AJ:6:ILE:HD11    | 10:AJ:72:VAL:CB    | 2.05                     | 0.83              |
| 35:BA:965:C:C5'     | 35:BA:2273:A:H1'   | 2.09                     | 0.83              |
| 38:BD:131:LEU:N     | 38:BD:131:LEU:HD12 | 1.94                     | 0.83              |
| 50:BR:117:VAL:O     | 50:BR:118:GLU:HB2  | 1.79                     | 0.83              |
| 52:BT:132:LYS:HD3   | 52:BT:132:LYS:H    | 1.41                     | 0.83              |
| 12:CL:90:VAL:O      | 12:CL:92:ASP:N     | 2.12                     | 0.83              |
| 24:CY:131:PRO:HG2   | 24:CY:281:PRO:HG3  | 1.60                     | 0.83              |
| 35:DA:1747(A):G:H2' | 35:DA:1748:G:C5'   | 2.09                     | 0.83              |
| 39:DE:24:THR:HG23   | 39:DE:184:VAL:HG23 | 1.61                     | 0.83              |
| 54:DV:21:ARG:HB3    | 54:DV:91:TYR:CD1   | 2.14                     | 0.83              |
| 16:CP:20:VAL:HG21   | 16:CP:32:TYR:CB    | 2.08                     | 0.82              |
| 40:DF:113:ALA:HB1   | 40:DF:186:ILE:HG21 | 1.61                     | 0.82              |
| 40:DF:40:GLN:NE2    | 40:DF:182:ASN:HB2  | 1.93                     | 0.82              |
| 51:DS:101:LEU:O     | 51:DS:101:LEU:HD12 | 1.77                     | 0.82              |
| 35:BA:218:A:C2      | 35:BA:235:U:H4'    | 2.13                     | 0.82              |
| 1:CA:1236:A:H2'     | 1:CA:1237:C:C6     | 2.14                     | 0.82              |
| 10:CJ:37:PRO:HA     | 10:CJ:72:VAL:HG22  | 1.59                     | 0.82              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:CM:15:VAL:HG12  | 13:CM:45:VAL:HG22  | 1.58                     | 0.82              |
| 24:CY:413:ILE:HG22 | 24:CY:449:THR:O    | 1.79                     | 0.82              |
| 24:CY:546:ILE:HD13 | 24:CY:565:VAL:HG11 | 1.60                     | 0.82              |
| 40:DF:64:ILE:HG22  | 40:DF:76:GLY:O     | 1.79                     | 0.82              |
| 2:AB:126:GLU:HA    | 2:AB:129:GLU:OE1   | 1.78                     | 0.82              |
| 24:AY:149:VAL:O    | 24:AY:152:THR:HG22 | 1.79                     | 0.82              |
| 31:B6:54:ILE:O     | 31:B6:54:ILE:HD12  | 1.79                     | 0.82              |
| 52:BT:65:LYS:HE3   | 52:BT:66:VAL:N     | 1.95                     | 0.82              |
| 58:BZ:79:ARG:O     | 58:BZ:80:ARG:HB2   | 1.77                     | 0.82              |
| 1:CA:1219:U:H2'    | 1:CA:1220:G:H8     | 1.43                     | 0.82              |
| 11:CK:124:LYS:HD2  | 11:CK:125:PHE:CE1  | 2.13                     | 0.82              |
| 35:DA:1314:C:H6    | 35:DA:1314:C:H5'   | 1.44                     | 0.82              |
| 35:DA:1947:C:C2'   | 35:DA:1948:G:H5''  | 2.08                     | 0.82              |
| 35:DA:2138:C:H2'   | 35:DA:2139:C:C6    | 2.13                     | 0.82              |
| 35:DA:2645:G:H4'   | 35:DA:2732:G:O2'   | 1.78                     | 0.82              |
| 35:DA:2394:C:OP1   | 48:DP:63:PRO:HD2   | 1.79                     | 0.82              |
| 5:AE:101:ILE:H     | 5:AE:101:ILE:HD13  | 1.45                     | 0.82              |
| 10:AJ:49:VAL:HG23  | 14:AN:41:ARG:HB2   | 1.61                     | 0.82              |
| 13:AM:124:PRO:HG2  | 24:AY:574:GLU:H    | 1.44                     | 0.82              |
| 35:BA:2787:C:H1'   | 39:BE:61:ARG:HG3   | 1.61                     | 0.82              |
| 49:BQ:30:GLY:HA2   | 49:BQ:107:ALA:HB2  | 1.61                     | 0.82              |
| 47:BO:104:ARG:HE   | 52:BT:33:LYS:HE3   | 1.44                     | 0.82              |
| 54:BV:21:ARG:HB3   | 54:BV:91:TYR:CD1   | 2.14                     | 0.82              |
| 58:BZ:151:HIS:HB3  | 58:BZ:170:THR:HA   | 1.59                     | 0.82              |
| 35:DA:1658:C:H2'   | 35:DA:1659:U:H6    | 1.43                     | 0.82              |
| 38:DD:91:ARG:HG2   | 38:DD:91:ARG:HH11  | 1.44                     | 0.82              |
| 1:AA:1510:U:H2'    | 1:AA:1511:G:C8     | 2.14                     | 0.82              |
| 35:BA:978:G:H1     | 35:BA:985:C:H42    | 1.24                     | 0.82              |
| 38:BD:44:ASN:CB    | 38:BD:49:ILE:HA    | 2.09                     | 0.82              |
| 40:BF:7:TYR:HD2    | 40:BF:16:GLY:HA3   | 1.43                     | 0.82              |
| 48:BP:40:SER:O     | 48:BP:41:ARG:HD2   | 1.77                     | 0.82              |
| 39:BE:111:ARG:HG3  | 50:BR:2:ARG:HG2    | 1.62                     | 0.82              |
| 52:BT:23:ARG:HG2   | 52:BT:120:ARG:NH1  | 1.95                     | 0.82              |
| 35:DA:598:G:H5'    | 48:DP:15:ARG:HB2   | 1.58                     | 0.82              |
| 48:DP:27:HIS:HD2   | 48:DP:28:GLY:N     | 1.76                     | 0.82              |
| 55:DW:29:LEU:HD11  | 55:DW:51:LEU:HD11  | 1.61                     | 0.82              |
| 25:B0:47:PRO:HG3   | 25:B0:59:LEU:HD21  | 1.59                     | 0.82              |
| 1:CA:1284:C:H3'    | 1:CA:1285:A:H5''   | 1.61                     | 0.82              |
| 1:CA:1342:C:H4'    | 9:CI:125:TYR:HB3   | 1.60                     | 0.82              |
| 22:CW:11:A:H2'     | 22:CW:12:G:H8      | 1.43                     | 0.82              |
| 44:DK:59:ILE:HG12  | 44:DK:60:TYR:N     | 1.95                     | 0.82              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 28:B3:17:LYS:NZ     | 28:B3:20:LYS:HE3  | 1.94                     | 0.82              |
| 35:BA:621:A:H2'     | 35:BA:622:G:H5'   | 1.62                     | 0.82              |
| 40:BF:155:LEU:HA    | 40:BF:174:VAL:HB  | 1.62                     | 0.82              |
| 44:BK:93:ARG:HB2    | 58:BZ:112:ARG:HE  | 1.43                     | 0.82              |
| 56:BX:12:VAL:HG12   | 56:BX:27:THR:O    | 1.79                     | 0.82              |
| 1:CA:1277:C:H2'     | 1:CA:1278:U:H5'   | 1.60                     | 0.82              |
| 35:DA:1884:A:C2'    | 35:DA:1885:A:H5'' | 2.10                     | 0.82              |
| 39:DE:24:THR:HG22   | 39:DE:186:GLY:HA2 | 1.61                     | 0.82              |
| 57:DY:46:LYS:H      | 57:DY:62:GLU:HB2  | 1.43                     | 0.82              |
| 1:AA:1489:G:C2'     | 1:AA:1490:C:H5''  | 2.09                     | 0.82              |
| 2:AB:29:ALA:O       | 2:AB:32:ILE:HG22  | 1.78                     | 0.82              |
| 35:BA:1884:A:C2'    | 35:BA:1885:A:H5'' | 2.09                     | 0.82              |
| 35:BA:2138:C:H2'    | 35:BA:2139:C:C6   | 2.13                     | 0.82              |
| 35:BA:2584:U:C2'    | 35:BA:2585:U:H5'  | 2.09                     | 0.82              |
| 54:BV:38:LEU:O      | 54:BV:39:LEU:HD13 | 1.80                     | 0.82              |
| 2:CB:12:GLU:O       | 2:CB:14:GLY:N     | 2.12                     | 0.82              |
| 10:CJ:6:ILE:HG22    | 10:CJ:98:ILE:HD12 | 1.62                     | 0.82              |
| 52:DT:23:ARG:HG2    | 52:DT:120:ARG:NH1 | 1.95                     | 0.82              |
| 3:AC:83:ARG:O       | 3:AC:86:VAL:HG22  | 1.80                     | 0.82              |
| 35:BA:2314:C:O2'    | 35:BA:2315:G:H5'  | 1.79                     | 0.82              |
| 35:BA:2473:U:H3'    | 35:BA:2474:C:C5'  | 2.08                     | 0.82              |
| 41:BG:171:ALA:O     | 41:BG:175:LEU:HG  | 1.80                     | 0.82              |
| 35:BA:1142(A):A:H4' | 46:BN:25:ARG:HH22 | 1.45                     | 0.82              |
| 48:BP:125:VAL:O     | 48:BP:145:PRO:HD2 | 1.78                     | 0.82              |
| 50:BR:10:LEU:HB3    | 50:BR:17:ARG:HD3  | 1.59                     | 0.82              |
| 52:BT:32:TYR:CD2    | 52:BT:32:TYR:N    | 2.48                     | 0.82              |
| 25:D0:11:ARG:HB2    | 25:D0:11:ARG:NH1  | 1.95                     | 0.82              |
| 35:DA:2439:A:O2'    | 35:DA:2587:A:H5'' | 1.80                     | 0.82              |
| 58:DZ:111:VAL:O     | 58:DZ:112:ARG:HB2 | 1.78                     | 0.82              |
| 10:AJ:6:ILE:O       | 10:AJ:6:ILE:HD12  | 1.78                     | 0.82              |
| 24:AY:555:LEU:HD21  | 24:AY:599:PRO:CG  | 2.10                     | 0.82              |
| 31:B6:14:THR:O      | 31:B6:49:HIS:HA   | 1.79                     | 0.82              |
| 35:BA:1485:G:H1'    | 35:BA:1505:C:H42  | 1.45                     | 0.82              |
| 35:BA:2524:G:H8     | 35:BA:2524:G:H5'  | 1.43                     | 0.82              |
| 39:BE:36:ARG:HG2    | 39:BE:36:ARG:HH11 | 1.42                     | 0.82              |
| 40:BF:64:ILE:HG22   | 40:BF:76:GLY:O    | 1.80                     | 0.82              |
| 57:BY:79:CYS:SG     | 57:BY:80:GLY:N    | 2.50                     | 0.82              |
| 1:CA:1053:G:N7      | 1:CA:1200:C:H5''  | 1.95                     | 0.82              |
| 35:DA:806:C:OP2     | 48:DP:39:LYS:HD3  | 1.79                     | 0.82              |
| 42:DH:30:LYS:HD2    | 42:DH:81:GLU:HG2  | 1.62                     | 0.82              |
| 13:AM:15:VAL:HG12   | 13:AM:45:VAL:HG22 | 1.62                     | 0.81              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:AX:19:U:H5'    | 24:AY:504:ARG:HB3 | 1.59                     | 0.81              |
| 25:B0:14:ARG:NH1  | 25:B0:14:ARG:HB2  | 1.95                     | 0.81              |
| 31:B6:28:ARG:HB3  | 31:B6:28:ARG:HH11 | 1.44                     | 0.81              |
| 35:BA:2585:U:O2'  | 35:BA:2586:C:H5'  | 1.80                     | 0.81              |
| 38:BD:24:ILE:HD13 | 38:BD:25:THR:H    | 1.45                     | 0.81              |
| 53:BU:34:LYS:HA   | 53:BU:34:LYS:HE2  | 1.60                     | 0.81              |
| 3:CC:20:SER:HB3   | 3:CC:40:ARG:NH2   | 1.95                     | 0.81              |
| 35:DA:288:C:H2'   | 35:DA:289:A:H8    | 1.44                     | 0.81              |
| 51:DS:13:ARG:HG3  | 51:DS:14:VAL:N    | 1.95                     | 0.81              |
| 52:DT:55:ASN:N    | 52:DT:59:THR:HG22 | 1.95                     | 0.81              |
| 5:AE:64:ARG:HG3   | 5:AE:64:ARG:HH11  | 1.45                     | 0.81              |
| 12:AL:41:ARG:HG2  | 12:AL:42:THR:H    | 1.44                     | 0.81              |
| 12:AL:90:VAL:O    | 12:AL:92:ASP:N    | 2.13                     | 0.81              |
| 38:BD:27:THR:CG2  | 38:BD:83:GLU:HG2  | 2.10                     | 0.81              |
| 1:CA:1364:U:O2    | 1:CA:1364:U:H2'   | 1.80                     | 0.81              |
| 11:CK:33:THR:HG22 | 11:CK:39:PRO:HA   | 1.62                     | 0.81              |
| 1:CA:1014:A:H4'   | 19:CS:14:HIS:CE1  | 2.15                     | 0.81              |
| 24:CY:92:ILE:HG23 | 24:CY:93:GLU:N    | 1.94                     | 0.81              |
| 52:DT:28:VAL:CG2  | 52:DT:46:GLU:HG3  | 2.10                     | 0.81              |
| 53:DU:31:SER:HB3  | 53:DU:34:LYS:HB2  | 1.61                     | 0.81              |
| 1:AA:1026:G:H2'   | 1:AA:1027:C:H5'   | 1.62                     | 0.81              |
| 9:AI:95:LYS:NZ    | 9:AI:96:LEU:HD12  | 1.95                     | 0.81              |
| 25:B0:40:GLN:NE2  | 25:B0:43:THR:HA   | 1.95                     | 0.81              |
| 36:BB:91:C:OP1    | 49:BQ:16:ARG:HG3  | 1.80                     | 0.81              |
| 25:D0:50:ASN:HA   | 25:D0:62:LEU:HD12 | 1.60                     | 0.81              |
| 26:D1:26:ARG:HG3  | 26:D1:27:GLU:HG3  | 1.62                     | 0.81              |
| 31:D6:14:THR:O    | 31:D6:49:HIS:HA   | 1.79                     | 0.81              |
| 35:DA:833:U:H5''  | 48:DP:48:PRO:HB3  | 1.61                     | 0.81              |
| 27:D2:2:LYS:HB2   | 35:DA:97:C:H5''   | 1.62                     | 0.81              |
| 39:DE:36:ARG:HG2  | 39:DE:36:ARG:HH11 | 1.43                     | 0.81              |
| 41:DG:38:VAL:HG13 | 41:DG:93:THR:HG23 | 1.62                     | 0.81              |
| 1:AA:1277:C:H2'   | 1:AA:1278:U:H5'   | 1.60                     | 0.81              |
| 2:AB:12:GLU:O     | 2:AB:14:GLY:N     | 2.13                     | 0.81              |
| 8:AH:83:ILE:HD12  | 8:AH:137:VAL:HG22 | 1.62                     | 0.81              |
| 30:B5:55:ARG:C    | 30:B5:55:ARG:HD3  | 1.99                     | 0.81              |
| 31:B6:19:ARG:HG2  | 35:BA:2400:G:O5'  | 1.80                     | 0.81              |
| 47:BO:24:VAL:HG21 | 47:BO:30:ALA:HB3  | 1.61                     | 0.81              |
| 52:BT:65:LYS:HA   | 52:BT:65:LYS:NZ   | 1.96                     | 0.81              |
| 52:BT:89:VAL:CG1  | 52:BT:91:ARG:HG3  | 2.10                     | 0.81              |
| 1:CA:1490:C:H5'   | 1:CA:1490:C:H6    | 1.46                     | 0.81              |
| 3:CC:175:LEU:HD21 | 3:CC:201:TYR:HE2  | 1.45                     | 0.81              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:CY:491:VAL:HG12 | 24:CY:492:ASP:N    | 1.96                     | 0.81              |
| 27:D2:38:GLN:O     | 27:D2:41:ILE:HG12  | 1.79                     | 0.81              |
| 38:DD:27:THR:CG2   | 38:DD:83:GLU:HG2   | 2.09                     | 0.81              |
| 18:AR:37:VAL:HG23  | 18:AR:38:GLU:N     | 1.96                     | 0.81              |
| 24:AY:21:ILE:H     | 24:AY:21:ILE:HD13  | 1.43                     | 0.81              |
| 35:BA:6:A:O2'      | 46:BN:130:HIS:HB2  | 1.79                     | 0.81              |
| 35:BA:833:U:H5''   | 48:BP:48:PRO:HB3   | 1.61                     | 0.81              |
| 41:BG:45:GLU:O     | 41:BG:51:ARG:HD3   | 1.80                     | 0.81              |
| 10:CJ:9:ARG:HG2    | 10:CJ:69:ASN:OD1   | 1.77                     | 0.81              |
| 33:D8:33:ASN:N     | 33:D8:33:ASN:HD22  | 1.77                     | 0.81              |
| 35:DA:2473:U:H3'   | 35:DA:2474:C:C5'   | 2.08                     | 0.81              |
| 37:DC:111:PHE:HE1  | 37:DC:137:LEU:HD13 | 1.46                     | 0.81              |
| 35:DA:2787:C:H1'   | 39:DE:61:ARG:HG3   | 1.61                     | 0.81              |
| 47:DO:43:VAL:HG23  | 47:DO:56:ASP:O     | 1.79                     | 0.81              |
| 36:DB:7:G:H5'      | 51:DS:29:PHE:CE1   | 2.15                     | 0.81              |
| 8:AH:89:PRO:HA     | 8:AH:92:ARG:NH1    | 1.96                     | 0.81              |
| 10:AJ:6:ILE:HG22   | 10:AJ:98:ILE:HD12  | 1.59                     | 0.81              |
| 26:B1:56:GLN:HA    | 26:B1:56:GLN:HE21  | 1.46                     | 0.81              |
| 46:BN:62:VAL:HG22  | 46:BN:66:LYS:HG3   | 1.62                     | 0.81              |
| 1:CA:975:A:H5'     | 1:CA:975:A:H8      | 1.44                     | 0.81              |
| 24:CY:578:SER:HB3  | 24:CY:581:ALA:HB2  | 1.62                     | 0.81              |
| 31:D6:48:VAL:HG23  | 31:D6:49:HIS:N     | 1.96                     | 0.81              |
| 35:DA:2585:U:O2'   | 35:DA:2586:C:H5'   | 1.80                     | 0.81              |
| 40:DF:155:LEU:HA   | 40:DF:174:VAL:HB   | 1.61                     | 0.81              |
| 52:DT:89:VAL:CG1   | 52:DT:91:ARG:HG3   | 2.10                     | 0.81              |
| 53:DU:34:LYS:HE2   | 53:DU:34:LYS:HA    | 1.61                     | 0.81              |
| 35:BA:1779:U:H5    | 35:BA:1784:A:N7    | 1.76                     | 0.81              |
| 35:BA:2126:A:H4'   | 35:BA:2127:G:O5'   | 1.80                     | 0.81              |
| 47:DO:114:ILE:HD12 | 47:DO:114:ILE:H    | 1.45                     | 0.81              |
| 48:DP:6:LEU:HB3    | 48:DP:9:ASN:ND2    | 1.95                     | 0.81              |
| 58:DZ:145:GLU:O    | 58:DZ:147:GLY:N    | 2.12                     | 0.81              |
| 27:B2:2:LYS:HD2    | 27:B2:5:GLU:OE1    | 1.81                     | 0.81              |
| 35:BA:1314:C:H5'   | 35:BA:1314:C:H6    | 1.44                     | 0.81              |
| 38:BD:91:ARG:HH11  | 38:BD:91:ARG:HG2   | 1.44                     | 0.81              |
| 41:BG:172:LEU:HD23 | 41:BG:176:LEU:HD11 | 1.63                     | 0.81              |
| 1:CA:1129:C:O2'    | 1:CA:1130:A:C8     | 2.33                     | 0.81              |
| 29:D4:53:GLU:HB3   | 29:D4:55:ARG:NE    | 1.96                     | 0.81              |
| 31:D6:28:ARG:HB3   | 31:D6:28:ARG:HH11  | 1.42                     | 0.81              |
| 31:D6:54:ILE:O     | 31:D6:54:ILE:HD12  | 1.81                     | 0.81              |
| 35:DA:2761:G:C2'   | 35:DA:2762:G:H5''  | 2.10                     | 0.81              |
| 35:DA:2778:A:H5'   | 35:DA:2779:U:OP2   | 1.81                     | 0.81              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:AB:31:TYR:HE1    | 2:AB:200:ILE:HD12 | 1.46                     | 0.81              |
| 9:AI:79:LEU:HD13   | 9:AI:83:ARG:HB2   | 1.63                     | 0.81              |
| 3:AC:6:HIS:ND1     | 14:AN:49:HIS:HB3  | 1.96                     | 0.81              |
| 30:B5:41:PRO:HG2   | 30:B5:44:THR:OG1  | 1.81                     | 0.81              |
| 26:D1:45:ASN:HD21  | 35:DA:2090:G:H21  | 1.29                     | 0.81              |
| 35:DA:2389:G:H5''  | 35:DA:2390:U:H5'  | 1.62                     | 0.81              |
| 42:DH:98:LEU:HB2   | 42:DH:125:VAL:CG2 | 2.06                     | 0.81              |
| 50:DR:4:LEU:O      | 50:DR:4:LEU:HD13  | 1.81                     | 0.81              |
| 42:BH:171:LEU:HD23 | 42:BH:172:LYS:O   | 1.79                     | 0.81              |
| 35:BA:598:G:H5'    | 48:BP:15:ARG:HB2  | 1.60                     | 0.81              |
| 54:BV:40:LEU:HA    | 54:BV:45:THR:HB   | 1.63                     | 0.81              |
| 3:CC:152:ILE:HG22  | 3:CC:167:TRP:HA   | 1.62                     | 0.81              |
| 9:CI:95:LYS:HZ3    | 9:CI:96:LEU:HD12  | 1.45                     | 0.81              |
| 18:CR:37:VAL:HG23  | 18:CR:38:GLU:N    | 1.96                     | 0.81              |
| 38:DD:35:LYS:HG3   | 38:DD:63:ARG:HG3  | 1.63                     | 0.81              |
| 52:DT:65:LYS:HA    | 52:DT:65:LYS:NZ   | 1.95                     | 0.81              |
| 5:AE:102:ALA:HB2   | 5:AE:120:THR:OG1  | 1.81                     | 0.81              |
| 35:BA:1541:G:H1'   | 35:BA:1542:A:C4   | 2.16                     | 0.81              |
| 46:BN:129:PRO:O    | 46:BN:130:HIS:HB3 | 1.80                     | 0.81              |
| 24:CY:548:GLU:OE1  | 24:CY:583:LYS:HE2 | 1.80                     | 0.81              |
| 24:CY:5:VAL:HG13   | 24:CY:6:GLU:H     | 1.46                     | 0.81              |
| 30:D5:40:LYS:NZ    | 30:D5:46:CYS:H    | 1.78                     | 0.81              |
| 42:DH:19:VAL:HG12  | 42:DH:20:ALA:H    | 1.46                     | 0.81              |
| 51:DS:65:VAL:O     | 51:DS:69:VAL:HG12 | 1.79                     | 0.81              |
| 1:AA:1318:A:H1'    | 19:AS:37:ARG:NH2  | 1.95                     | 0.80              |
| 25:B0:11:ARG:HB2   | 25:B0:11:ARG:NH1  | 1.96                     | 0.80              |
| 35:BA:1059:G:H2'   | 35:BA:1060:U:C5   | 2.16                     | 0.80              |
| 44:BK:93:ARG:CB    | 58:BZ:112:ARG:HE  | 1.94                     | 0.80              |
| 51:BS:89:ARG:HG3   | 51:BS:92:TYR:CA   | 2.11                     | 0.80              |
| 53:BU:44:ASN:HD21  | 54:BV:75:PHE:HB3  | 1.47                     | 0.80              |
| 4:CD:49:ARG:HE     | 4:CD:49:ARG:HA    | 1.44                     | 0.80              |
| 24:CY:92:ILE:CG1   | 24:CY:405:PRO:HG2 | 2.11                     | 0.80              |
| 35:DA:1541:G:H1'   | 35:DA:1542:A:C4   | 2.17                     | 0.80              |
| 35:DA:9:U:H5       | 35:DA:2629:A:H62  | 1.27                     | 0.80              |
| 35:DA:2804:C:H2'   | 35:DA:2805:G:C8   | 2.16                     | 0.80              |
| 1:AA:299:G:H2'     | 1:AA:300:A:C8     | 2.16                     | 0.80              |
| 24:AY:21:ILE:HG13  | 35:BA:2661:G:H5'' | 1.61                     | 0.80              |
| 25:B0:43:THR:H     | 35:BA:2331:G:H4'  | 1.45                     | 0.80              |
| 41:BG:172:LEU:O    | 41:BG:176:LEU:HG  | 1.82                     | 0.80              |
| 50:BR:4:LEU:O      | 50:BR:4:LEU:HD13  | 1.81                     | 0.80              |
| 51:BS:13:ARG:CG    | 51:BS:14:VAL:H    | 1.94                     | 0.80              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 2:CB:121:LEU:HD22   | 2:CB:126:GLU:HB2   | 1.63                     | 0.80              |
| 52:DT:29:ARG:HB3    | 52:DT:85:LYS:HA    | 1.62                     | 0.80              |
| 1:AA:1053:G:N7      | 1:AA:1200:C:H5''   | 1.95                     | 0.80              |
| 35:BA:979:G:H3'     | 35:BA:980:A:C5'    | 2.11                     | 0.80              |
| 42:BH:83:TYR:HB3    | 42:BH:134:SER:HA   | 1.61                     | 0.80              |
| 24:AY:662:LYS:NZ    | 42:BH:175:LYS:HG3  | 1.96                     | 0.80              |
| 48:BP:57:THR:OG1    | 48:BP:59:LEU:HB3   | 1.81                     | 0.80              |
| 5:CE:101:ILE:H      | 5:CE:101:ILE:HD13  | 1.46                     | 0.80              |
| 9:CI:79:LEU:HD13    | 9:CI:83:ARG:HB2    | 1.63                     | 0.80              |
| 1:AA:148:G:H2'      | 1:AA:149:A:C8      | 2.17                     | 0.80              |
| 1:AA:438:G:H4'      | 1:AA:439:A:OP1     | 1.79                     | 0.80              |
| 1:AA:625:G:H2'      | 1:AA:626:U:H6      | 1.47                     | 0.80              |
| 7:AG:45:ASP:O       | 7:AG:49:ILE:HG12   | 1.80                     | 0.80              |
| 1:AA:1342:C:H4'     | 9:AI:125:TYR:HB3   | 1.63                     | 0.80              |
| 48:BP:23:PRO:HB2    | 48:BP:33:ARG:HG3   | 1.61                     | 0.80              |
| 24:CY:530:VAL:HG22  | 24:CY:531:GLY:H    | 1.45                     | 0.80              |
| 35:DA:965:C:C5'     | 35:DA:2273:A:H1'   | 2.11                     | 0.80              |
| 35:DA:2483:C:H3'    | 35:DA:2484:G:H5''  | 1.64                     | 0.80              |
| 35:DA:970:C:H2'     | 35:DA:971:C:H6     | 1.45                     | 0.80              |
| 41:DG:5:VAL:HB      | 41:DG:8:LYS:HB2    | 1.64                     | 0.80              |
| 50:DR:73:VAL:O      | 50:DR:76:VAL:HG12  | 1.80                     | 0.80              |
| 51:DS:89:ARG:HG3    | 51:DS:92:TYR:CA    | 2.10                     | 0.80              |
| 29:B4:53:GLU:HB3    | 29:B4:55:ARG:HE    | 1.47                     | 0.80              |
| 35:BA:1539:G:C2     | 35:BA:1540:U:H1'   | 2.16                     | 0.80              |
| 41:BG:61:ALA:HA     | 41:BG:64:THR:HG22  | 1.64                     | 0.80              |
| 24:AY:662:LYS:HZ2   | 42:BH:175:LYS:CD   | 1.94                     | 0.80              |
| 1:CA:1495:U:H2'     | 1:CA:1496:C:C6     | 2.16                     | 0.80              |
| 8:CH:89:PRO:HA      | 8:CH:92:ARG:NH1    | 1.97                     | 0.80              |
| 24:CY:228:MET:O     | 24:CY:232:LEU:HD22 | 1.82                     | 0.80              |
| 35:DA:1142(A):A:H2' | 35:DA:1143:A:H5''  | 1.62                     | 0.80              |
| 35:DA:203:C:H3'     | 35:DA:204:A:H5''   | 1.62                     | 0.80              |
| 38:DD:147:LEU:HD13  | 38:DD:155:LEU:HD11 | 1.63                     | 0.80              |
| 41:DG:46:ALA:HB2    | 41:DG:88:ILE:CB    | 2.12                     | 0.80              |
| 39:DE:111:ARG:HG3   | 50:DR:2:ARG:HG2    | 1.64                     | 0.80              |
| 52:DT:53:ARG:HH11   | 52:DT:53:ARG:HB3   | 1.47                     | 0.80              |
| 44:BK:59:ILE:HG12   | 44:BK:60:TYR:N     | 1.95                     | 0.80              |
| 1:CA:438:G:H4'      | 1:CA:439:A:OP1     | 1.80                     | 0.80              |
| 32:D7:19:ARG:HD3    | 35:DA:125:G:H5'    | 1.63                     | 0.80              |
| 35:DA:1539:G:C2     | 35:DA:1540:U:H1'   | 2.17                     | 0.80              |
| 32:D7:41:ARG:HH22   | 35:DA:460:A:P      | 2.04                     | 0.80              |
| 12:AL:6:THR:HG23    | 12:AL:9:GLN:HE21   | 1.46                     | 0.80              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:AY:513:LYS:CB   | 24:AY:566:THR:HB   | 2.11                     | 0.80              |
| 30:B5:40:LYS:NZ    | 30:B5:46:CYS:H     | 1.79                     | 0.80              |
| 35:BA:2463:C:O2'   | 35:BA:2464:C:H5'   | 1.82                     | 0.80              |
| 1:CA:1363(A):A:H4' | 1:CA:1364:U:H5''   | 1.64                     | 0.80              |
| 5:CE:82:VAL:HG21   | 5:CE:138:ALA:HA    | 1.63                     | 0.80              |
| 29:D4:10:VAL:HG23  | 29:D4:11:PRO:HD2   | 1.61                     | 0.80              |
| 38:DD:44:ASN:CB    | 38:DD:49:ILE:HA    | 2.11                     | 0.80              |
| 40:DF:160:ASN:OD1  | 40:DF:163:VAL:HG23 | 1.81                     | 0.80              |
| 1:AA:662:G:H2'     | 1:AA:663:A:C8      | 2.17                     | 0.80              |
| 9:AI:114:TYR:HE1   | 10:AJ:60:ARG:H     | 1.24                     | 0.80              |
| 35:BA:226:G:H4'    | 35:BA:227:A:OP1    | 1.82                     | 0.80              |
| 35:BA:2761:G:C2'   | 35:BA:2762:G:H5''  | 2.11                     | 0.80              |
| 41:BG:135:LEU:HD11 | 41:BG:155:MET:CG   | 2.11                     | 0.80              |
| 52:BT:29:ARG:HB3   | 52:BT:85:LYS:HA    | 1.63                     | 0.80              |
| 58:BZ:42:VAL:HG13  | 58:BZ:43:GLU:H     | 1.45                     | 0.80              |
| 24:CY:193:GLY:HA3  | 24:CY:266:ASN:HB3  | 1.62                     | 0.80              |
| 49:DQ:6:ARG:O      | 49:DQ:7:MET:HG3    | 1.81                     | 0.80              |
| 54:DV:38:LEU:O     | 54:DV:39:LEU:HD13  | 1.80                     | 0.80              |
| 5:AE:82:VAL:HG21   | 5:AE:138:ALA:HA    | 1.64                     | 0.80              |
| 12:AL:25:PRO:C     | 12:AL:27:LEU:H     | 1.84                     | 0.80              |
| 24:AY:573:HIS:HD2  | 24:AY:576:ASP:H    | 1.28                     | 0.80              |
| 28:B3:29:ARG:HB2   | 28:B3:29:ARG:HH11  | 1.44                     | 0.80              |
| 35:BA:2518:A:H5''  | 35:BA:2519:U:OP2   | 1.81                     | 0.80              |
| 38:BD:35:LYS:HG3   | 38:BD:63:ARG:HG3   | 1.64                     | 0.80              |
| 40:BF:160:ASN:OD1  | 40:BF:163:VAL:HG23 | 1.82                     | 0.80              |
| 40:BF:28:ILE:HD13  | 40:BF:28:ILE:H     | 1.47                     | 0.80              |
| 44:BK:77:LEU:H     | 44:BK:77:LEU:HD23  | 1.45                     | 0.80              |
| 58:BZ:86:VAL:HG12  | 58:BZ:87:ASP:H     | 1.46                     | 0.80              |
| 1:CA:1026:G:H2'    | 1:CA:1027:C:H5'    | 1.62                     | 0.80              |
| 27:D2:12:GLU:O     | 27:D2:16:LEU:HG    | 1.82                     | 0.80              |
| 27:D2:24:LEU:HD22  | 27:D2:60:LEU:HD11  | 1.63                     | 0.80              |
| 35:DA:2189:U:C2'   | 35:DA:2190:G:H5''  | 2.12                     | 0.80              |
| 38:DD:24:ILE:HD13  | 38:DD:25:THR:H     | 1.46                     | 0.80              |
| 1:AA:1219:U:H2'    | 1:AA:1220:G:H8     | 1.47                     | 0.80              |
| 1:AA:1497:G:O2'    | 1:AA:1498:U:H5'    | 1.81                     | 0.80              |
| 9:AI:88:TYR:O      | 9:AI:89:ASN:HB2    | 1.81                     | 0.80              |
| 31:B6:37:ARG:NH1   | 35:BA:2286:A:N7    | 2.29                     | 0.80              |
| 48:BP:6:LEU:HB3    | 48:BP:9:ASN:ND2    | 1.96                     | 0.80              |
| 51:BS:65:VAL:O     | 51:BS:69:VAL:HG12  | 1.81                     | 0.80              |
| 1:CA:1489:G:H2'    | 1:CA:1490:C:C5'    | 2.11                     | 0.80              |
| 2:CB:126:GLU:HA    | 2:CB:129:GLU:OE1   | 1.80                     | 0.80              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 22:CW:6:G:H2'       | 22:CW:7:G:O4'     | 1.82                     | 0.80              |
| 35:DA:1947:C:H2'    | 35:DA:1948:G:H5'' | 1.62                     | 0.80              |
| 42:DH:83:TYR:HB3    | 42:DH:134:SER:HA  | 1.62                     | 0.80              |
| 47:DO:104:ARG:HE    | 52:DT:33:LYS:HE3  | 1.47                     | 0.80              |
| 53:DU:88:ILE:HG22   | 54:DV:47:VAL:O    | 1.82                     | 0.80              |
| 58:DZ:53:ILE:HG22   | 58:DZ:71:VAL:HB   | 1.64                     | 0.80              |
| 1:AA:1435:G:H2'     | 1:AA:1436:U:C6    | 2.18                     | 0.79              |
| 24:AY:227:ILE:HG23  | 24:AY:237:PRO:HG2 | 1.63                     | 0.79              |
| 35:BA:212:G:H8      | 35:BA:212:G:H5'   | 1.46                     | 0.79              |
| 1:CA:1442:G:C6      | 1:CA:1442(B):A:H2 | 2.00                     | 0.79              |
| 2:CB:204:ASN:HD22   | 2:CB:205:ASP:N    | 1.80                     | 0.79              |
| 2:CB:97:TRP:HZ2     | 2:CB:102:LEU:HD13 | 1.45                     | 0.79              |
| 35:DA:107:C:H2'     | 35:DA:108:U:C6    | 2.17                     | 0.79              |
| 35:DA:212:G:H5'     | 35:DA:212:G:H8    | 1.45                     | 0.79              |
| 35:DA:861:A:H2'     | 35:DA:862:G:O4'   | 1.82                     | 0.79              |
| 37:DC:31:LYS:HE3    | 37:DC:179:ALA:O   | 1.82                     | 0.79              |
| 50:DR:63:ARG:HH22   | 50:DR:77:ARG:HG2  | 1.47                     | 0.79              |
| 53:DU:44:ASN:HD21   | 54:DV:75:PHE:HB3  | 1.47                     | 0.79              |
| 55:DW:59:VAL:HG12   | 55:DW:59:VAL:O    | 1.83                     | 0.79              |
| 2:AB:97:TRP:HZ2     | 2:AB:102:LEU:HD13 | 1.46                     | 0.79              |
| 38:BD:83:GLU:HB2    | 38:BD:92:ILE:HD11 | 1.64                     | 0.79              |
| 51:BS:49:VAL:HG12   | 51:BS:50:SER:H    | 1.46                     | 0.79              |
| 4:CD:96:LEU:H       | 4:CD:96:LEU:HD22  | 1.47                     | 0.79              |
| 35:DA:979:G:H3'     | 35:DA:980:A:C5'   | 2.10                     | 0.79              |
| 42:DH:85:LYS:NZ     | 42:DH:87:LEU:HG   | 1.96                     | 0.79              |
| 44:DK:4:VAL:HG12    | 44:DK:5:VAL:H     | 1.45                     | 0.79              |
| 56:DX:53:LYS:HD2    | 56:DX:55:ASN:HD21 | 1.48                     | 0.79              |
| 58:DZ:108:PRO:HA    | 58:DZ:142:SER:HA  | 1.64                     | 0.79              |
| 1:AA:1129:C:O2'     | 1:AA:1130:A:C8    | 2.34                     | 0.79              |
| 35:BA:2068:U:N3     | 35:BA:2430:A:H2   | 1.80                     | 0.79              |
| 42:BH:98:LEU:HB2    | 42:BH:125:VAL:CG2 | 2.08                     | 0.79              |
| 48:BP:102:ARG:HB3   | 48:BP:102:ARG:NH2 | 1.98                     | 0.79              |
| 48:BP:77:ARG:HB2    | 48:BP:78:PRO:HD2  | 1.64                     | 0.79              |
| 1:CA:148:G:H2'      | 1:CA:149:A:C8     | 2.16                     | 0.79              |
| 1:CA:243:A:H4'      | 1:CA:244:U:O5'    | 1.80                     | 0.79              |
| 3:CC:150:LYS:HB2    | 3:CC:169:ALA:CB   | 2.12                     | 0.79              |
| 25:D0:43:THR:H      | 35:DA:2331:G:H4'  | 1.45                     | 0.79              |
| 44:DK:59:ILE:HG12   | 44:DK:60:TYR:H    | 1.47                     | 0.79              |
| 58:DZ:163:LEU:HD23  | 58:DZ:163:LEU:H   | 1.47                     | 0.79              |
| 33:B8:48:PHE:O      | 33:B8:49:VAL:HG13 | 1.82                     | 0.79              |
| 35:BA:1142(A):A:H2' | 35:BA:1143:A:H5'' | 1.62                     | 0.79              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 35:BA:2804:C:H2'   | 35:BA:2805:G:C8     | 2.17                     | 0.79              |
| 41:BG:91:ARG:HD2   | 41:BG:92:VAL:N      | 1.96                     | 0.79              |
| 42:BH:19:VAL:HG12  | 42:BH:20:ALA:H      | 1.46                     | 0.79              |
| 52:BT:53:ARG:HH11  | 52:BT:53:ARG:HB3    | 1.46                     | 0.79              |
| 5:CE:81:GLU:HG2    | 5:CE:90:VAL:HG22    | 1.65                     | 0.79              |
| 34:D9:32:HIS:O     | 34:D9:34:GLN:HG3    | 1.82                     | 0.79              |
| 35:DA:1541:G:H4'   | 35:DA:1542:A:O5'    | 1.83                     | 0.79              |
| 46:DN:129:PRO:O    | 46:DN:130:HIS:HB3   | 1.79                     | 0.79              |
| 48:DP:30:THR:HG22  | 48:DP:31:ALA:N      | 1.98                     | 0.79              |
| 52:DT:80:SER:HB3   | 52:DT:81:PRO:HD3    | 1.64                     | 0.79              |
| 58:DZ:145:GLU:C    | 58:DZ:147:GLY:H     | 1.86                     | 0.79              |
| 24:AY:122:TRP:CE3  | 24:AY:132:ARG:HD2   | 2.18                     | 0.79              |
| 41:BG:16:ARG:HE    | 41:BG:31:VAL:HG11   | 1.48                     | 0.79              |
| 42:BH:41:MET:CG    | 42:BH:43:VAL:HG13   | 2.11                     | 0.79              |
| 42:BH:85:LYS:NZ    | 42:BH:87:LEU:HG     | 1.97                     | 0.79              |
| 49:BQ:54:MET:HG2   | 49:BQ:64:ILE:HD13   | 1.64                     | 0.79              |
| 53:BU:53:ARG:HA    | 53:BU:56:ASP:OD2    | 1.83                     | 0.79              |
| 57:BY:7:VAL:HB     | 57:BY:8:LYS:CD      | 2.11                     | 0.79              |
| 1:CA:662:G:H2'     | 1:CA:663:A:C8       | 2.18                     | 0.79              |
| 31:D6:43:CYS:HB2   | 31:D6:44:ARG:HH21   | 1.48                     | 0.79              |
| 42:DH:41:MET:CG    | 42:DH:43:VAL:HG13   | 2.13                     | 0.79              |
| 48:DP:115:LEU:HA   | 48:DP:134:ALA:HB3   | 1.63                     | 0.79              |
| 24:AY:466:LEU:HA   | 24:AY:470:PHE:CD2   | 2.18                     | 0.79              |
| 35:BA:2389:G:H5''  | 35:BA:2390:U:H5'    | 1.65                     | 0.79              |
| 35:BA:861:A:H2'    | 35:BA:862:G:O4'     | 1.82                     | 0.79              |
| 52:BT:80:SER:HB3   | 52:BT:81:PRO:HD3    | 1.62                     | 0.79              |
| 12:CL:25:PRO:C     | 12:CL:27:LEU:H      | 1.86                     | 0.79              |
| 12:CL:41:ARG:HG2   | 12:CL:42:THR:H      | 1.48                     | 0.79              |
| 35:DA:1494:A:C2'   | 35:DA:1495:A:H5''   | 2.12                     | 0.79              |
| 35:DA:272(G):C:C2' | 35:DA:272(H):C:H5'' | 2.12                     | 0.79              |
| 35:DA:621:A:H2'    | 35:DA:622:G:H5'     | 1.63                     | 0.79              |
| 1:AA:182:U:H5'     | 1:AA:183:G:OP2      | 1.83                     | 0.79              |
| 13:AM:68:GLY:N     | 13:AM:71:ARG:HB3    | 1.97                     | 0.79              |
| 31:B6:43:CYS:HB2   | 31:B6:44:ARG:HH21   | 1.48                     | 0.79              |
| 32:B7:41:ARG:HH22  | 35:BA:460:A:P       | 2.05                     | 0.79              |
| 33:B8:62:LEU:HD13  | 35:BA:242:G:H5''    | 1.63                     | 0.79              |
| 35:BA:288:C:H2'    | 35:BA:289:A:H8      | 1.45                     | 0.79              |
| 44:BK:59:ILE:HG12  | 44:BK:60:TYR:H      | 1.48                     | 0.79              |
| 48:BP:30:THR:HG22  | 48:BP:31:ALA:N      | 1.97                     | 0.79              |
| 3:CC:34:LEU:HD22   | 3:CC:38:ARG:HD2     | 1.65                     | 0.79              |
| 3:CC:6:HIS:ND1     | 14:CN:49:HIS:HB3    | 1.98                     | 0.79              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:2584:U:C2'   | 35:DA:2585:U:H5'   | 2.11                     | 0.79              |
| 35:DA:299:A:H5'    | 35:DA:300:A:OP2    | 1.82                     | 0.79              |
| 35:BA:533:G:H5''   | 53:BU:24:TYR:CD2   | 2.17                     | 0.79              |
| 39:BE:1:MET:HB3    | 39:BE:200:GLU:OE1  | 1.83                     | 0.79              |
| 40:BF:113:ALA:HB1  | 40:BF:186:ILE:HG21 | 1.65                     | 0.79              |
| 44:BK:81:ALA:HB1   | 44:BK:99:ILE:HD11  | 1.63                     | 0.79              |
| 51:BS:13:ARG:HG3   | 51:BS:14:VAL:N     | 1.97                     | 0.79              |
| 1:CA:328:C:H2'     | 1:CA:328:C:O2      | 1.83                     | 0.79              |
| 24:CY:491:VAL:HG12 | 24:CY:492:ASP:H    | 1.46                     | 0.79              |
| 27:D2:69:ARG:HG3   | 27:D2:70:GLN:H     | 1.48                     | 0.79              |
| 53:DU:110:VAL:HG12 | 53:DU:114:LYS:HD3  | 1.63                     | 0.79              |
| 56:DX:53:LYS:HD2   | 56:DX:55:ASN:ND2   | 1.97                     | 0.79              |
| 1:AA:625:G:H2'     | 1:AA:626:U:C6      | 2.18                     | 0.79              |
| 24:AY:505:GLY:HA3  | 24:AY:576:ASP:CG   | 2.03                     | 0.79              |
| 35:BA:107:C:H2'    | 35:BA:108:U:C6     | 2.18                     | 0.79              |
| 35:BA:2189:U:C2'   | 35:BA:2190:G:H5''  | 2.12                     | 0.79              |
| 7:CG:4:ARG:HB3     | 7:CG:5:ARG:HH11    | 1.47                     | 0.79              |
| 13:CM:68:GLY:N     | 13:CM:71:ARG:HB3   | 1.97                     | 0.79              |
| 33:D8:62:LEU:HD13  | 35:DA:242:G:H5''   | 1.63                     | 0.79              |
| 44:DK:81:ALA:HB1   | 44:DK:99:ILE:HD11  | 1.63                     | 0.79              |
| 46:DN:57:ALA:H     | 46:DN:124:ALA:HA   | 1.46                     | 0.79              |
| 1:AA:814:A:H2'     | 1:AA:816:A:H5'     | 1.63                     | 0.79              |
| 24:AY:196:ILE:O    | 24:AY:197:ARG:HB2  | 1.83                     | 0.79              |
| 24:AY:91:THR:O     | 24:AY:93:GLU:N     | 2.16                     | 0.79              |
| 35:BA:1259:G:O2'   | 35:BA:1260:G:H5'   | 1.83                     | 0.79              |
| 35:BA:1845:G:H2'   | 35:BA:1846:G:C5'   | 2.12                     | 0.79              |
| 1:CA:1490:C:C6     | 1:CA:1490:C:H5'    | 2.18                     | 0.79              |
| 1:CA:182:U:H5'     | 1:CA:183:G:OP2     | 1.83                     | 0.79              |
| 10:CJ:32:ALA:HB2   | 10:CJ:76:ASN:HD22  | 1.47                     | 0.79              |
| 41:DG:34:LEU:H     | 41:DG:34:LEU:HD12  | 1.48                     | 0.79              |
| 52:DT:118:ARG:HA   | 52:DT:121:ILE:HB   | 1.65                     | 0.79              |
| 58:DZ:7:ALA:O      | 58:DZ:62:PRO:HD3   | 1.82                     | 0.79              |
| 14:AN:41:ARG:HG2   | 14:AN:41:ARG:HH11  | 1.47                     | 0.78              |
| 24:AY:427:ALA:HB1  | 24:AY:466:LEU:CD1  | 2.12                     | 0.78              |
| 35:BA:1375:C:H2'   | 35:BA:1376:C:H6    | 1.48                     | 0.78              |
| 35:BA:2439:A:O2'   | 35:BA:2587:A:H5''  | 1.83                     | 0.78              |
| 44:BK:100:THR:HA   | 44:BK:139:VAL:HB   | 1.65                     | 0.78              |
| 24:CY:65:ILE:O     | 24:CY:65:ILE:HG12  | 1.82                     | 0.78              |
| 35:DA:2122:U:H2'   | 35:DA:2123:G:C8    | 2.18                     | 0.78              |
| 35:DA:2076:U:H5'   | 35:DA:2238:G:H22   | 1.48                     | 0.78              |
| 35:DA:2476:A:C2'   | 35:DA:2477:C:H5''  | 2.13                     | 0.78              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:DP:77:ARG:HB2  | 48:DP:78:PRO:HD2   | 1.63                     | 0.78              |
| 56:DX:12:VAL:HB   | 56:DX:17:ALA:CB    | 2.09                     | 0.78              |
| 10:AJ:7:LYS:HB2   | 10:AJ:97:GLU:HB2   | 1.63                     | 0.78              |
| 24:AY:157:LEU:N   | 24:AY:157:LEU:HD23 | 1.97                     | 0.78              |
| 26:B1:5:CYS:SG    | 26:B1:62:VAL:HA    | 2.22                     | 0.78              |
| 35:BA:299:A:H5'   | 35:BA:300:A:OP2    | 1.82                     | 0.78              |
| 36:BB:87:G:C3'    | 36:BB:88:C:H5''    | 2.13                     | 0.78              |
| 56:BX:53:LYS:HD2  | 56:BX:55:ASN:HD21  | 1.47                     | 0.78              |
| 35:DA:2514:U:H2'  | 35:DA:2515:C:H6    | 1.49                     | 0.78              |
| 49:DQ:54:MET:HG2  | 49:DQ:64:ILE:HD13  | 1.65                     | 0.78              |
| 1:AA:797:C:OP1    | 11:AK:124:LYS:HE3  | 1.83                     | 0.78              |
| 10:AJ:4:ILE:HD13  | 10:AJ:74:ILE:HG13  | 1.66                     | 0.78              |
| 13:AM:66:LEU:HD12 | 13:AM:66:LEU:N     | 1.97                     | 0.78              |
| 15:AO:80:ALA:HB1  | 15:AO:84:LYS:HE2   | 1.66                     | 0.78              |
| 33:B8:33:ASN:N    | 33:B8:33:ASN:HD22  | 1.79                     | 0.78              |
| 35:BA:904:C:H5'   | 35:BA:904:C:H6     | 1.47                     | 0.78              |
| 22:CW:7:G:H5''    | 22:CW:50:G:OP2     | 1.84                     | 0.78              |
| 38:DD:95:LEU:HD12 | 38:DD:103:ARG:O    | 1.83                     | 0.78              |
| 42:DH:83:TYR:HB3  | 42:DH:135:GLY:H    | 1.49                     | 0.78              |
| 50:DR:2:ARG:HD2   | 50:DR:5:LYS:HE2    | 1.65                     | 0.78              |
| 11:AK:33:THR:HG22 | 11:AK:39:PRO:HA    | 1.64                     | 0.78              |
| 27:B2:69:ARG:HH22 | 35:BA:111:A:C4'    | 1.96                     | 0.78              |
| 35:BA:142:A:H8    | 35:BA:1595:G:H21   | 1.31                     | 0.78              |
| 37:BC:111:PHE:HE1 | 37:BC:137:LEU:HD13 | 1.48                     | 0.78              |
| 58:BZ:77:ASP:O    | 58:BZ:79:ARG:N     | 2.15                     | 0.78              |
| 7:CG:45:ASP:O     | 7:CG:49:ILE:HG12   | 1.84                     | 0.78              |
| 24:CY:191:ASP:HB3 | 24:CY:265:LYS:HD2  | 1.65                     | 0.78              |
| 31:D6:19:ARG:HG2  | 35:DA:2400:G:O5'   | 1.81                     | 0.78              |
| 36:DB:103:G:H21   | 58:DZ:73:GLN:NE2   | 1.81                     | 0.78              |
| 42:DH:85:LYS:HE3  | 42:DH:145:ALA:HB1  | 1.66                     | 0.78              |
| 2:AB:121:LEU:HD22 | 2:AB:126:GLU:HB2   | 1.65                     | 0.78              |
| 9:AI:26:VAL:HG22  | 9:AI:61:ALA:HB3    | 1.64                     | 0.78              |
| 9:AI:95:LYS:HD3   | 9:AI:96:LEU:N      | 1.98                     | 0.78              |
| 12:AL:27:LEU:O    | 12:AL:29:GLY:N     | 2.15                     | 0.78              |
| 35:BA:1434:A:H61  | 35:BA:1558:A:N6    | 1.81                     | 0.78              |
| 41:BG:87:PRO:O    | 41:BG:88:ILE:HD12  | 1.83                     | 0.78              |
| 24:CY:9:LEU:HD23  | 24:CY:9:LEU:O      | 1.82                     | 0.78              |
| 29:D4:56:VAL:HG12 | 29:D4:56:VAL:O     | 1.82                     | 0.78              |
| 33:D8:48:PHE:O    | 33:D8:49:VAL:HG13  | 1.83                     | 0.78              |
| 38:DD:83:GLU:HB2  | 38:DD:92:ILE:HD11  | 1.65                     | 0.78              |
| 1:AA:509:A:C5'    | 1:AA:510:A:OP2     | 2.30                     | 0.78              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:AC:152:ILE:HG22 | 3:AC:167:TRP:HA    | 1.65                     | 0.78              |
| 23:AX:15:A:H5'    | 23:AX:16:A:OP1     | 1.83                     | 0.78              |
| 28:B3:17:LYS:HZ3  | 28:B3:20:LYS:HE3   | 1.48                     | 0.78              |
| 29:B4:53:GLU:HB3  | 29:B4:55:ARG:NE    | 1.98                     | 0.78              |
| 35:BA:2476:A:C2'  | 35:BA:2477:C:H5''  | 2.13                     | 0.78              |
| 24:AY:662:LYS:HZ3 | 42:BH:175:LYS:HG3  | 1.47                     | 0.78              |
| 50:BR:2:ARG:HD2   | 50:BR:5:LYS:HE2    | 1.66                     | 0.78              |
| 53:BU:91:ASP:OD1  | 53:BU:96:ALA:HB2   | 1.84                     | 0.78              |
| 26:D1:24:ALA:HB2  | 26:D1:32:LYS:HE3   | 1.66                     | 0.78              |
| 35:DA:1538:G:H2'  | 35:DA:1539:G:C8    | 2.18                     | 0.78              |
| 38:DD:144:ALA:HB3 | 38:DD:192:THR:HG23 | 1.66                     | 0.78              |
| 39:DE:50:GLY:HA2  | 39:DE:78:LEU:HB3   | 1.66                     | 0.78              |
| 54:DV:46:VAL:HG22 | 54:DV:47:VAL:H     | 1.49                     | 0.78              |
| 4:AD:13:ARG:O     | 4:AD:15:GLU:N      | 2.17                     | 0.78              |
| 56:BX:53:LYS:HD2  | 56:BX:55:ASN:ND2   | 1.98                     | 0.78              |
| 1:CA:1438:G:H2'   | 1:CA:1439:C:H6     | 1.46                     | 0.78              |
| 10:CJ:6:ILE:HD12  | 10:CJ:6:ILE:O      | 1.82                     | 0.78              |
| 35:DA:1845:G:H2'  | 35:DA:1846:G:C5'   | 2.14                     | 0.78              |
| 31:D6:37:ARG:NH1  | 35:DA:2286:A:N7    | 2.32                     | 0.78              |
| 36:DB:66:A:H61    | 36:DB:108:U:H2'    | 1.47                     | 0.78              |
| 41:DG:76:SER:CB   | 41:DG:83:ARG:HB3   | 2.13                     | 0.78              |
| 35:DA:1007:C:H4'  | 46:DN:108:PRO:HD3  | 1.66                     | 0.78              |
| 50:DR:21:TYR:HB3  | 50:DR:47:PHE:CD2   | 2.19                     | 0.78              |
| 30:D5:27:PRO:HG3  | 55:DW:23:LEU:HD11  | 1.66                     | 0.78              |
| 1:AA:1037:C:H2'   | 1:AA:1038:C:C2     | 2.19                     | 0.78              |
| 8:AH:10:LEU:HD22  | 8:AH:83:ILE:HD11   | 1.65                     | 0.78              |
| 24:AY:201:ILE:H   | 24:AY:201:ILE:HD12 | 1.49                     | 0.78              |
| 24:AY:380:LEU:C   | 24:AY:381:LYS:HD2  | 2.04                     | 0.78              |
| 35:BA:545:C:C2'   | 35:BA:547:A:H5''   | 2.14                     | 0.78              |
| 40:BF:157:VAL:CG2 | 40:BF:194:MET:HG2  | 2.13                     | 0.78              |
| 52:BT:55:ASN:N    | 52:BT:59:THR:HG22  | 1.98                     | 0.78              |
| 10:CJ:49:VAL:O    | 10:CJ:60:ARG:HB3   | 1.83                     | 0.78              |
| 39:DE:1:MET:HB3   | 39:DE:200:GLU:OE1  | 1.84                     | 0.78              |
| 42:DH:149:ARG:HD3 | 42:DH:164:TYR:CE1  | 2.19                     | 0.78              |
| 54:DV:18:LEU:HD22 | 54:DV:19:LYS:N     | 1.97                     | 0.78              |
| 1:AA:1238:A:H5'   | 1:AA:1336:C:N4     | 1.97                     | 0.78              |
| 4:AD:96:LEU:H     | 4:AD:96:LEU:HD22   | 1.48                     | 0.78              |
| 48:BP:91:PHE:H    | 48:BP:91:PHE:HD1   | 1.28                     | 0.78              |
| 52:BT:13:ARG:HA   | 52:BT:13:ARG:NH1   | 1.99                     | 0.78              |
| 1:CA:1369:C:H2'   | 1:CA:1370:G:C8     | 2.18                     | 0.78              |
| 29:D4:53:GLU:HB3  | 29:D4:55:ARG:HE    | 1.46                     | 0.78              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 30:D5:44:THR:HG22  | 30:D5:45:VAL:H    | 1.49                     | 0.78              |
| 35:DA:1188:U:O2'   | 35:DA:1189:A:H5'  | 1.83                     | 0.78              |
| 35:DA:1434:A:H61   | 35:DA:1558:A:N6   | 1.81                     | 0.78              |
| 35:DA:2518:A:H5''  | 35:DA:2519:U:OP2  | 1.84                     | 0.78              |
| 48:DP:91:PHE:HD1   | 48:DP:91:PHE:H    | 1.30                     | 0.78              |
| 35:BA:1188:U:O2'   | 35:BA:1189:A:H5'  | 1.84                     | 0.78              |
| 42:BH:13:LYS:HA    | 42:BH:13:LYS:HE2  | 1.66                     | 0.78              |
| 48:BP:115:LEU:HA   | 48:BP:134:ALA:HB3 | 1.64                     | 0.78              |
| 20:CT:57:ARG:NH1   | 20:CT:102:GLY:HA2 | 1.99                     | 0.78              |
| 24:CY:230:LYS:NZ   | 24:CY:237:PRO:HA  | 1.98                     | 0.78              |
| 35:DA:1115:G:H2'   | 35:DA:1116:C:C6   | 2.19                     | 0.78              |
| 1:AA:1225:A:N3     | 1:AA:1225:A:H2'   | 1.99                     | 0.77              |
| 3:AC:46:GLU:O      | 3:AC:47:LEU:HB2   | 1.83                     | 0.77              |
| 3:AC:70:VAL:O      | 3:AC:106:VAL:HG23 | 1.83                     | 0.77              |
| 7:AG:4:ARG:HB3     | 7:AG:5:ARG:HH11   | 1.47                     | 0.77              |
| 10:AJ:40:LEU:N     | 10:AJ:40:LEU:HD23 | 1.99                     | 0.77              |
| 20:AT:57:ARG:NH1   | 20:AT:102:GLY:HA2 | 1.99                     | 0.77              |
| 35:BA:1538:G:H2'   | 35:BA:1539:G:C8   | 2.18                     | 0.77              |
| 35:BA:2514:U:H2'   | 35:BA:2515:C:H6   | 1.48                     | 0.77              |
| 35:BA:556:G:H2'    | 35:BA:557:U:C6    | 2.19                     | 0.77              |
| 40:BF:3:GLU:HA     | 40:BF:24:LEU:CG   | 2.13                     | 0.77              |
| 42:BH:170:ARG:O    | 42:BH:171:LEU:HB3 | 1.84                     | 0.77              |
| 53:BU:47:TYR:HA    | 53:BU:50:ARG:NH2  | 1.99                     | 0.77              |
| 55:BW:59:VAL:HG12  | 55:BW:59:VAL:O    | 1.82                     | 0.77              |
| 1:CA:1037:C:H2'    | 1:CA:1038:C:C2    | 2.18                     | 0.77              |
| 1:CA:447:G:H2'     | 1:CA:485:G:N2     | 1.99                     | 0.77              |
| 9:CI:26:VAL:HG22   | 9:CI:61:ALA:HB3   | 1.65                     | 0.77              |
| 10:CJ:4:ILE:HD13   | 10:CJ:74:ILE:HG13 | 1.65                     | 0.77              |
| 22:CV:21:A:H61     | 22:CV:46:G:H2'    | 1.47                     | 0.77              |
| 24:CY:238:THR:HG23 | 24:CY:241:GLU:H   | 1.48                     | 0.77              |
| 24:CY:84:THR:H     | 24:CY:85:PRO:CD   | 1.97                     | 0.77              |
| 27:D2:69:ARG:HH22  | 35:DA:111:A:C5'   | 1.97                     | 0.77              |
| 35:DA:1578:U:H2'   | 35:DA:1579:A:H5'' | 1.66                     | 0.77              |
| 35:DA:2657:A:H2'   | 35:DA:2658:C:H5'  | 1.65                     | 0.77              |
| 35:DA:83:G:HO2'    | 35:DA:84:A:H8     | 1.31                     | 0.77              |
| 36:DB:87:G:C3'     | 36:DB:88:C:H5''   | 2.14                     | 0.77              |
| 42:DH:175:LYS:O    | 42:DH:176:ALA:CB  | 2.32                     | 0.77              |
| 4:AD:114:ARG:HG3   | 4:AD:114:ARG:HH11 | 1.48                     | 0.77              |
| 10:AJ:9:ARG:HG2    | 10:AJ:69:ASN:OD1  | 1.84                     | 0.77              |
| 11:AK:111:ASP:OD2  | 18:AR:84:LYS:HE2  | 1.83                     | 0.77              |
| 35:BA:2020:A:C2'   | 35:BA:2021:C:H5'' | 2.14                     | 0.77              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 35:BA:2262:U:H2'   | 35:BA:2263:C:C5'    | 2.15                     | 0.77              |
| 36:BB:66:A:H61     | 36:BB:108:U:H2'     | 1.48                     | 0.77              |
| 35:BA:1243:G:H1'   | 48:BP:8:PRO:HB3     | 1.65                     | 0.77              |
| 1:CA:1270:C:H2'    | 1:CA:1271:G:C8      | 2.19                     | 0.77              |
| 35:DA:2463:C:O2'   | 35:DA:2464:C:H5'    | 1.84                     | 0.77              |
| 35:DA:2577:A:H5'   | 35:DA:2578:G:H5'    | 1.65                     | 0.77              |
| 1:AA:328:C:O2      | 1:AA:328:C:H2'      | 1.84                     | 0.77              |
| 22:AV:46:G:H4'     | 22:AV:47:U:C5       | 2.15                     | 0.77              |
| 26:B1:76:ARG:NH1   | 26:B1:95:LEU:HD22   | 1.99                     | 0.77              |
| 35:BA:395:U:H2'    | 35:BA:396:G:C8      | 2.19                     | 0.77              |
| 58:BZ:4:ARG:HH12   | 58:BZ:66:SER:HB2    | 1.50                     | 0.77              |
| 3:CC:70:VAL:O      | 3:CC:106:VAL:HG23   | 1.84                     | 0.77              |
| 9:CI:104:ARG:O     | 9:CI:104:ARG:HG2    | 1.82                     | 0.77              |
| 9:CI:95:LYS:NZ     | 9:CI:96:LEU:HD12    | 1.99                     | 0.77              |
| 30:D5:58:LEU:O     | 30:D5:58:LEU:HD22   | 1.85                     | 0.77              |
| 35:DA:2126:A:H4'   | 35:DA:2127:G:O5'    | 1.82                     | 0.77              |
| 35:DA:533:G:H5''   | 53:DU:24:TYR:CD2    | 2.19                     | 0.77              |
| 44:DK:93:ARG:CB    | 58:DZ:112:ARG:HE    | 1.97                     | 0.77              |
| 10:AJ:32:ALA:HB2   | 10:AJ:76:ASN:HD22   | 1.49                     | 0.77              |
| 13:AM:99:ARG:O     | 13:AM:101:GLN:HG3   | 1.84                     | 0.77              |
| 35:BA:272(G):C:C2' | 35:BA:272(H):C:H5'' | 2.14                     | 0.77              |
| 53:BU:88:ILE:HG22  | 54:BV:47:VAL:O      | 1.84                     | 0.77              |
| 54:BV:18:LEU:HD22  | 54:BV:19:LYS:N      | 1.99                     | 0.77              |
| 4:CD:13:ARG:O      | 4:CD:15:GLU:N       | 2.17                     | 0.77              |
| 10:CJ:96:ILE:H     | 10:CJ:96:ILE:HD13   | 1.48                     | 0.77              |
| 22:CW:31:G:H2'     | 22:CW:32:G:H8       | 1.50                     | 0.77              |
| 35:DA:154(A):C:C5' | 35:DA:155:U:H5''    | 2.13                     | 0.77              |
| 35:DA:82:G:H5''    | 35:DA:296:C:H5'     | 1.65                     | 0.77              |
| 40:DF:20:LEU:HD22  | 40:DF:23:ASP:OD2    | 1.83                     | 0.77              |
| 48:DP:102:ARG:HB3  | 48:DP:102:ARG:NH2   | 1.99                     | 0.77              |
| 53:DU:47:TYR:HA    | 53:DU:50:ARG:NH2    | 1.99                     | 0.77              |
| 56:DX:27:THR:HB    | 56:DX:80:ILE:HG22   | 1.66                     | 0.77              |
| 3:AC:150:LYS:HB2   | 3:AC:169:ALA:CB     | 2.14                     | 0.77              |
| 22:AV:46:G:O3'     | 22:AV:47:U:H6       | 1.68                     | 0.77              |
| 29:B4:56:VAL:O     | 29:B4:56:VAL:HG12   | 1.83                     | 0.77              |
| 35:BA:871:U:H4'    | 49:BQ:69:PHE:CE2    | 2.20                     | 0.77              |
| 53:BU:110:VAL:HG12 | 53:BU:114:LYS:HD3   | 1.67                     | 0.77              |
| 58:BZ:59:LEU:O     | 58:BZ:66:SER:HA     | 1.84                     | 0.77              |
| 4:CD:114:ARG:HG3   | 4:CD:114:ARG:HH11   | 1.48                     | 0.77              |
| 4:CD:152:SER:O     | 4:CD:155:LEU:HG     | 1.85                     | 0.77              |
| 12:CL:20:LYS:H     | 12:CL:20:LYS:HD3    | 1.49                     | 0.77              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:DA:1223:G:H3'   | 35:DA:1224:C:C5'  | 2.14                     | 0.77              |
| 35:DA:2334:G:H5'   | 51:DS:13:ARG:HD3  | 1.67                     | 0.77              |
| 35:DA:364:C:H2'    | 35:DA:365:C:H5''  | 1.66                     | 0.77              |
| 27:D2:47:ASN:HB2   | 35:DA:95:G:H1'    | 1.65                     | 0.77              |
| 42:DH:66:GLY:HA2   | 42:DH:69:ARG:HB3  | 1.66                     | 0.77              |
| 51:DS:49:VAL:HG12  | 51:DS:50:SER:H    | 1.49                     | 0.77              |
| 56:DX:12:VAL:HG12  | 56:DX:27:THR:O    | 1.83                     | 0.77              |
| 24:AY:169:GLY:HA3  | 24:AY:173:THR:O   | 1.85                     | 0.77              |
| 35:BA:1348:G:C2'   | 35:BA:1349:A:H5'' | 2.14                     | 0.77              |
| 35:BA:1578:U:H2'   | 35:BA:1579:A:H5'' | 1.65                     | 0.77              |
| 7:CG:151:TYR:OH    | 11:CK:54:ARG:HD3  | 1.85                     | 0.77              |
| 12:CL:6:THR:HG23   | 12:CL:9:GLN:HE21  | 1.49                     | 0.77              |
| 24:CY:128:TYR:O    | 24:CY:129:LYS:HB2 | 1.83                     | 0.77              |
| 24:CY:174:PHE:CZ   | 24:CY:261:GLY:HA2 | 2.20                     | 0.77              |
| 35:DA:1434:A:H61   | 35:DA:1558:A:H62  | 1.31                     | 0.77              |
| 41:DG:121:ASN:CB   | 41:DG:124:SER:HB2 | 2.14                     | 0.77              |
| 44:DK:100:THR:HA   | 44:DK:139:VAL:HB  | 1.66                     | 0.77              |
| 35:DA:1243:G:H1'   | 48:DP:8:PRO:HB3   | 1.64                     | 0.77              |
| 53:DU:53:ARG:HA    | 53:DU:56:ASP:OD2  | 1.84                     | 0.77              |
| 54:DV:58:VAL:O     | 54:DV:97:LYS:HB2  | 1.84                     | 0.77              |
| 1:AA:559:A:H4'     | 1:AA:560:U:H5'    | 1.66                     | 0.77              |
| 24:AY:199:ILE:HD12 | 24:AY:199:ILE:O   | 1.85                     | 0.77              |
| 29:B4:13:ARG:HB3   | 29:B4:13:ARG:HH11 | 1.48                     | 0.77              |
| 35:BA:2657:A:H2'   | 35:BA:2658:C:H5'  | 1.66                     | 0.77              |
| 35:BA:2778:A:H5'   | 35:BA:2779:U:OP2  | 1.84                     | 0.77              |
| 38:BD:145:VAL:HG22 | 38:BD:191:ALA:HB1 | 1.64                     | 0.77              |
| 42:BH:171:LEU:HD23 | 42:BH:171:LEU:C   | 2.04                     | 0.77              |
| 46:BN:35:ARG:O     | 46:BN:37:LYS:N    | 2.17                     | 0.77              |
| 1:CA:1411:C:H2'    | 1:CA:1412:C:H6    | 1.50                     | 0.77              |
| 22:CV:17:C:H5''    | 22:CV:17(A):U:C6  | 2.17                     | 0.77              |
| 35:DA:1946:U:H2'   | 35:DA:1947:C:C6   | 2.19                     | 0.77              |
| 35:DA:904:C:H5'    | 35:DA:904:C:H6    | 1.47                     | 0.77              |
| 57:DY:7:VAL:HB     | 57:DY:8:LYS:CD    | 2.13                     | 0.77              |
| 58:DZ:37:VAL:O     | 58:DZ:38:TYR:HB3  | 1.85                     | 0.77              |
| 35:BA:1494:A:C2'   | 35:BA:1495:A:H5'' | 2.13                     | 0.77              |
| 35:BA:533:G:H5''   | 53:BU:24:TYR:CE2  | 2.20                     | 0.77              |
| 36:BB:112:U:H2'    | 36:BB:113:G:H8    | 1.49                     | 0.77              |
| 37:BC:90:ALA:HA    | 37:BC:155:ARG:NH1 | 2.00                     | 0.77              |
| 42:BH:153:LYS:HG3  | 42:BH:154:PRO:HD2 | 1.67                     | 0.77              |
| 46:BN:96:GLU:N     | 46:BN:96:GLU:OE2  | 2.18                     | 0.77              |
| 1:CA:1238:A:H5'    | 1:CA:1336:C:N4    | 1.99                     | 0.77              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1444:C:H2'    | 1:CA:1445:C:C6     | 2.19                     | 0.77              |
| 2:CB:31:TYR:HE1    | 2:CB:200:ILE:HD12  | 1.49                     | 0.77              |
| 35:DA:1053:C:C3'   | 35:DA:1054:A:H5''  | 2.15                     | 0.77              |
| 24:AY:180:VAL:HG23 | 24:AY:216:LEU:HD12 | 1.67                     | 0.77              |
| 30:B5:44:THR:HG22  | 30:B5:45:VAL:H     | 1.48                     | 0.77              |
| 52:BT:28:VAL:CG2   | 52:BT:46:GLU:HG3   | 2.15                     | 0.77              |
| 9:CI:17:VAL:HG11   | 9:CI:81:ILE:HD13   | 1.66                     | 0.77              |
| 16:CP:20:VAL:CG2   | 16:CP:32:TYR:HB2   | 2.14                     | 0.77              |
| 1:CA:275:G:H5''    | 17:CQ:14:LYS:HB2   | 1.67                     | 0.77              |
| 35:DA:2068:U:N3    | 35:DA:2430:A:H2    | 1.83                     | 0.77              |
| 35:DA:2103:C:C2'   | 35:DA:2104:G:H5''  | 2.14                     | 0.77              |
| 39:DE:47:VAL:HG12  | 39:DE:48:GLN:N     | 2.00                     | 0.77              |
| 40:DF:3:GLU:HA     | 40:DF:24:LEU:CG    | 2.12                     | 0.77              |
| 41:DG:77:ILE:HG22  | 41:DG:80:PHE:N     | 2.00                     | 0.77              |
| 46:DN:65:LYS:HB3   | 46:DN:69:GLN:HG3   | 1.67                     | 0.77              |
| 52:DT:83:ILE:HG13  | 52:DT:84:GLN:N     | 1.98                     | 0.77              |
| 57:DY:62:GLU:HG2   | 57:DY:63:LYS:H     | 1.50                     | 0.77              |
| 2:AB:22:LYS:H      | 2:AB:40:HIS:CE1    | 2.03                     | 0.77              |
| 19:AS:64:GLU:HG2   | 29:B4:48:ARG:NH2   | 2.00                     | 0.77              |
| 41:BG:68:PRO:CA    | 41:BG:92:VAL:HG12  | 2.12                     | 0.77              |
| 30:D5:41:PRO:HG2   | 30:D5:44:THR:OG1   | 1.85                     | 0.77              |
| 35:DA:226:G:H4'    | 35:DA:227:A:OP1    | 1.83                     | 0.77              |
| 37:DC:90:ALA:HA    | 37:DC:155:ARG:NH1  | 2.00                     | 0.77              |
| 42:DH:171:LEU:C    | 42:DH:171:LEU:HD23 | 2.04                     | 0.77              |
| 46:DN:35:ARG:O     | 46:DN:37:LYS:N     | 2.18                     | 0.77              |
| 53:DU:92:ARG:O     | 53:DU:94:ASN:N     | 2.18                     | 0.77              |
| 1:AA:1116:C:H2'    | 1:AA:1117:G:H5''   | 1.67                     | 0.76              |
| 2:AB:17:PHE:HB3    | 2:AB:44:LEU:HD21   | 1.67                     | 0.76              |
| 3:AC:3:ASN:O       | 3:AC:4:LYS:HB2     | 1.85                     | 0.76              |
| 9:AI:104:ARG:HG2   | 9:AI:104:ARG:O     | 1.84                     | 0.76              |
| 1:AA:1250:A:H4'    | 9:AI:68:GLY:H      | 1.50                     | 0.76              |
| 27:B2:69:ARG:HG3   | 27:B2:70:GLN:H     | 1.49                     | 0.76              |
| 40:BF:20:LEU:HD22  | 40:BF:23:ASP:OD2   | 1.84                     | 0.76              |
| 41:BG:55:LYS:O     | 41:BG:58:GLN:HG3   | 1.85                     | 0.76              |
| 41:BG:98:ARG:HH11  | 41:BG:98:ARG:HG2   | 1.48                     | 0.76              |
| 35:BA:1007:C:H4'   | 46:BN:108:PRO:HD3  | 1.67                     | 0.76              |
| 1:AA:1432:G:OP1    | 52:BT:107:ASP:HB2  | 1.85                     | 0.76              |
| 1:CA:309:G:H1'     | 1:CA:608:A:C2      | 2.20                     | 0.76              |
| 11:CK:58:PRO:HA    | 11:CK:90:GLY:HA3   | 1.67                     | 0.76              |
| 24:CY:331:TYR:O    | 24:CY:371:ALA:HB1  | 1.84                     | 0.76              |
| 19:CS:64:GLU:HG2   | 29:D4:48:ARG:NH2   | 2.00                     | 0.76              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:D6:27:LYS:HD2   | 31:D6:27:LYS:O     | 1.85                     | 0.76              |
| 38:DD:261:LYS:NZ   | 38:DD:263:ARG:HH12 | 1.83                     | 0.76              |
| 35:DA:871:U:H4'    | 49:DQ:69:PHE:CE2   | 2.20                     | 0.76              |
| 57:DY:2:ARG:HD3    | 57:DY:3:VAL:HG23   | 1.67                     | 0.76              |
| 58:DZ:166:SER:HB2  | 58:DZ:168:GLU:N    | 2.00                     | 0.76              |
| 24:AY:415:PRO:HA   | 24:AY:474:ALA:CB   | 2.14                     | 0.76              |
| 35:BA:2076:U:H5'   | 35:BA:2238:G:H22   | 1.47                     | 0.76              |
| 37:BC:31:LYS:HE3   | 37:BC:179:ALA:O    | 1.84                     | 0.76              |
| 42:BH:83:TYR:HB3   | 42:BH:135:GLY:H    | 1.48                     | 0.76              |
| 54:BV:45:THR:O     | 54:BV:46:VAL:HG12  | 1.85                     | 0.76              |
| 56:BX:8:ILE:H      | 56:BX:8:ILE:HD12   | 1.49                     | 0.76              |
| 57:BY:2:ARG:HD3    | 57:BY:3:VAL:HG23   | 1.67                     | 0.76              |
| 1:CA:179:A:H2'     | 1:CA:180:U:C6      | 2.20                     | 0.76              |
| 16:CP:25:ARG:HG3   | 16:CP:25:ARG:HH11  | 1.49                     | 0.76              |
| 22:CV:35:A:O2'     | 22:CV:36:U:H5'     | 1.85                     | 0.76              |
| 24:CY:630:GLN:NE2  | 24:CY:646:PHE:HD2  | 1.84                     | 0.76              |
| 35:DA:1689:A:H62   | 35:DA:1698:A:H2    | 1.29                     | 0.76              |
| 35:DA:2312:U:OP1   | 41:DG:73:ALA:HA    | 1.85                     | 0.76              |
| 35:DA:962:G:O2'    | 35:DA:963:U:H5'    | 1.84                     | 0.76              |
| 42:DH:170:ARG:O    | 42:DH:171:LEU:HB3  | 1.84                     | 0.76              |
| 1:AA:1270:C:H2'    | 1:AA:1271:G:C8     | 2.21                     | 0.76              |
| 3:AC:16:ARG:CB     | 3:AC:16:ARG:HH11   | 1.97                     | 0.76              |
| 24:AY:67:ALA:HB1   | 24:AY:327:PHE:CZ   | 2.19                     | 0.76              |
| 35:BA:1053:C:C3'   | 35:BA:1054:A:H5''  | 2.15                     | 0.76              |
| 35:BA:108:U:H2'    | 35:BA:109:G:H8     | 1.47                     | 0.76              |
| 35:BA:1517:G:H8    | 35:BA:1517:G:H5'   | 1.48                     | 0.76              |
| 35:BA:2483:C:H3'   | 35:BA:2484:G:H5''  | 1.66                     | 0.76              |
| 35:BA:979:G:H3'    | 35:BA:980:A:H5'    | 1.68                     | 0.76              |
| 37:BC:101:ILE:O    | 37:BC:105:LEU:HB2  | 1.85                     | 0.76              |
| 42:BH:85:LYS:HE3   | 42:BH:145:ALA:HB1  | 1.65                     | 0.76              |
| 1:CA:194:C:H2'     | 1:CA:195:A:H5''    | 1.66                     | 0.76              |
| 35:DA:1390:U:O2'   | 35:DA:1391:U:H5'   | 1.84                     | 0.76              |
| 35:DA:1409:C:H2'   | 35:DA:1410:G:H8    | 1.49                     | 0.76              |
| 35:DA:545:C:C2'    | 35:DA:547:A:H5''   | 2.15                     | 0.76              |
| 41:DG:138:GLN:HB3  | 41:DG:153:ARG:O    | 1.86                     | 0.76              |
| 51:DS:34:HIS:CE1   | 51:DS:54:LEU:HB3   | 2.20                     | 0.76              |
| 52:DT:13:ARG:NH1   | 52:DT:13:ARG:HA    | 2.00                     | 0.76              |
| 52:DT:32:TYR:CD2   | 52:DT:32:TYR:N     | 2.52                     | 0.76              |
| 55:DW:29:LEU:CD1   | 55:DW:51:LEU:HD11  | 2.15                     | 0.76              |
| 56:DX:12:VAL:HG12  | 56:DX:27:THR:HG23  | 1.67                     | 0.76              |
| 1:AA:1363(A):A:H4' | 1:AA:1364:U:H5''   | 1.66                     | 0.76              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:AB:204:ASN:HD22 | 2:AB:205:ASP:N     | 1.83                     | 0.76              |
| 6:AF:45:LEU:O     | 6:AF:46:ARG:HG3    | 1.84                     | 0.76              |
| 12:AL:20:LYS:H    | 12:AL:20:LYS:HD3   | 1.48                     | 0.76              |
| 35:BA:1541:G:H4'  | 35:BA:1542:A:O5'   | 1.83                     | 0.76              |
| 35:BA:2103:C:C2'  | 35:BA:2104:G:H5''  | 2.15                     | 0.76              |
| 35:BA:84:A:H5''   | 57:BY:9:LYS:NZ     | 2.00                     | 0.76              |
| 35:BA:907:U:OP1   | 49:BQ:24:GLY:N     | 2.18                     | 0.76              |
| 52:BT:83:ILE:HG13 | 52:BT:84:GLN:N     | 2.00                     | 0.76              |
| 58:BZ:40:ASP:OD1  | 58:BZ:42:VAL:HG12  | 1.86                     | 0.76              |
| 1:CA:625:G:H2'    | 1:CA:626:U:H6      | 1.50                     | 0.76              |
| 17:CQ:67:LYS:HA   | 17:CQ:70:ARG:HH12  | 1.50                     | 0.76              |
| 23:CX:12:A:H3'    | 23:CX:12:A:N3      | 2.00                     | 0.76              |
| 35:DA:1259:G:O2'  | 35:DA:1260:G:H5'   | 1.84                     | 0.76              |
| 39:DE:59:VAL:HG11 | 39:DE:63:LEU:HG    | 1.68                     | 0.76              |
| 52:DT:129:ARG:NH2 | 52:DT:130:ALA:HA   | 2.00                     | 0.76              |
| 52:DT:65:LYS:HE3  | 52:DT:66:VAL:N     | 1.98                     | 0.76              |
| 1:AA:631:G:H2'    | 1:AA:632:A:C8      | 2.21                     | 0.76              |
| 1:AA:792:A:O2'    | 1:AA:794:A:N7      | 2.18                     | 0.76              |
| 2:AB:124:SER:OG   | 2:AB:125:PRO:HD2   | 1.86                     | 0.76              |
| 35:BA:2334:G:H5'  | 51:BS:13:ARG:HD3   | 1.67                     | 0.76              |
| 35:BA:2789:C:H1'  | 35:BA:2892:A:C2    | 2.20                     | 0.76              |
| 36:BB:103:G:H5'   | 36:BB:104:U:OP2    | 1.85                     | 0.76              |
| 44:BK:17:ALA:CB   | 44:BK:38:VAL:HG22  | 2.16                     | 0.76              |
| 50:BR:63:ARG:HH22 | 50:BR:77:ARG:HG2   | 1.49                     | 0.76              |
| 53:BU:47:TYR:HA   | 53:BU:50:ARG:HH21  | 1.51                     | 0.76              |
| 58:BZ:115:GLY:N   | 58:BZ:177:PRO:HG3  | 2.01                     | 0.76              |
| 1:CA:1219:U:H2'   | 1:CA:1220:G:C8     | 2.20                     | 0.76              |
| 4:CD:98:GLU:HG2   | 4:CD:189:PRO:HG3   | 1.68                     | 0.76              |
| 1:CA:1250:A:H4'   | 9:CI:68:GLY:H      | 1.51                     | 0.76              |
| 24:CY:92:ILE:CG2  | 24:CY:93:GLU:H     | 1.99                     | 0.76              |
| 35:DA:2146:C:H4'  | 35:DA:2147:G:C8    | 2.21                     | 0.76              |
| 35:DA:218:A:H2    | 35:DA:235:U:H4'    | 1.51                     | 0.76              |
| 35:DA:2645:G:C3'  | 35:DA:2646:C:H5'   | 2.13                     | 0.76              |
| 35:DA:907:U:OP1   | 49:DQ:24:GLY:N     | 2.18                     | 0.76              |
| 54:DV:40:LEU:HA   | 54:DV:45:THR:HB    | 1.66                     | 0.76              |
| 1:AA:1236:A:H2'   | 1:AA:1237:C:C6     | 2.20                     | 0.76              |
| 1:AA:194:C:H2'    | 1:AA:195:A:H5''    | 1.67                     | 0.76              |
| 35:BA:82:G:H5''   | 35:BA:296:C:H5'    | 1.67                     | 0.76              |
| 44:BK:93:ARG:HB2  | 58:BZ:112:ARG:HH21 | 1.50                     | 0.76              |
| 1:CA:942:G:H21    | 9:CI:124:GLN:NE2   | 1.84                     | 0.76              |
| 13:CM:99:ARG:O    | 13:CM:101:GLN:HG3  | 1.86                     | 0.76              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:D5:3:LYS:HD2    | 30:D5:5:PRO:HD2    | 1.66                     | 0.76              |
| 35:DA:1348:G:C2'   | 35:DA:1349:A:H5''  | 2.14                     | 0.76              |
| 35:DA:1517:G:H8    | 35:DA:1517:G:H5'   | 1.51                     | 0.76              |
| 36:DB:82:G:O2'     | 36:DB:83:G:H5'     | 1.85                     | 0.76              |
| 41:DG:85:GLY:C     | 41:DG:87:PRO:HD3   | 2.06                     | 0.76              |
| 44:DK:17:ALA:HB3   | 44:DK:38:VAL:HG22  | 1.68                     | 0.76              |
| 53:DU:91:ASP:OD1   | 53:DU:96:ALA:HB2   | 1.86                     | 0.76              |
| 56:DX:8:ILE:H      | 56:DX:8:ILE:HD12   | 1.50                     | 0.76              |
| 1:AA:1030(D):A:H2' | 1:AA:1031:G:H5'    | 1.68                     | 0.76              |
| 3:AC:142:MET:HE2   | 3:AC:171:GLY:HA3   | 1.67                     | 0.76              |
| 4:AD:152:SER:O     | 4:AD:155:LEU:HG    | 1.85                     | 0.76              |
| 24:AY:21:ILE:HG21  | 24:AY:88:VAL:HG13  | 1.67                     | 0.76              |
| 31:B6:27:LYS:HB3   | 31:B6:32:ASN:ND2   | 2.01                     | 0.76              |
| 35:BA:1223:G:H3'   | 35:BA:1224:C:C5'   | 2.15                     | 0.76              |
| 35:BA:154(A):C:C5' | 35:BA:155:U:H5''   | 2.14                     | 0.76              |
| 35:BA:2807:G:H1    | 35:BA:2893:G:H1    | 1.33                     | 0.76              |
| 35:BA:654(S):G:H3' | 35:BA:654(T):C:C5' | 2.16                     | 0.76              |
| 49:BQ:59:ARG:HB3   | 58:BZ:180:VAL:HG21 | 1.67                     | 0.76              |
| 50:BR:21:TYR:HB3   | 50:BR:47:PHE:CD2   | 2.20                     | 0.76              |
| 1:CA:1225:A:H2'    | 1:CA:1225:A:N3     | 2.00                     | 0.76              |
| 5:CE:87:SER:HB3    | 5:CE:131:ILE:CD1   | 2.14                     | 0.76              |
| 1:CA:797:C:OP1     | 11:CK:124:LYS:HE3  | 1.86                     | 0.76              |
| 24:CY:592:GLU:HA   | 24:CY:595:GLN:HB2  | 1.68                     | 0.76              |
| 35:DA:2713:A:H3'   | 35:DA:2714:G:H5'   | 1.68                     | 0.76              |
| 35:DA:882:G:H2'    | 35:DA:883:G:C8     | 2.20                     | 0.76              |
| 38:DD:35:LYS:CG    | 38:DD:63:ARG:HG3   | 2.15                     | 0.76              |
| 1:AA:1239:A:H2'    | 1:AA:1298:C:H42    | 1.51                     | 0.76              |
| 33:B8:48:PHE:O     | 33:B8:49:VAL:HG22  | 1.85                     | 0.76              |
| 38:BD:44:ASN:HB2   | 38:BD:48:ARG:O     | 1.85                     | 0.76              |
| 41:BG:86:MET:N     | 41:BG:87:PRO:HD3   | 2.00                     | 0.76              |
| 42:BH:85:LYS:C     | 42:BH:85:LYS:HD3   | 2.06                     | 0.76              |
| 52:BT:115:ARG:HB3  | 52:BT:115:ARG:NH1  | 2.00                     | 0.76              |
| 1:CA:103:C:H3'     | 1:CA:104:G:H8      | 1.50                     | 0.76              |
| 3:CC:142:MET:HE2   | 3:CC:171:GLY:HA3   | 1.67                     | 0.76              |
| 13:CM:19:LEU:HB3   | 13:CM:25:ILE:HG21  | 1.68                     | 0.76              |
| 11:CK:111:ASP:OD2  | 18:CR:84:LYS:HE2   | 1.85                     | 0.76              |
| 24:CY:548:GLU:O    | 24:CY:551:GLN:HG2  | 1.85                     | 0.76              |
| 61:CY:702:FUA:C12  | 61:CY:702:FUA:H231 | 2.15                     | 0.76              |
| 26:D1:46:LEU:HD22  | 26:D1:46:LEU:N     | 2.01                     | 0.76              |
| 26:D1:86:SER:O     | 26:D1:90:ILE:HG12  | 1.85                     | 0.76              |
| 35:DA:1375:C:H2'   | 35:DA:1376:C:H6    | 1.50                     | 0.76              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:DC:101:ILE:O    | 37:DC:105:LEU:HB2  | 1.86                     | 0.76              |
| 42:DH:85:LYS:HD3   | 42:DH:85:LYS:C     | 2.06                     | 0.76              |
| 52:DT:38:ASN:C     | 52:DT:38:ASN:ND2   | 2.40                     | 0.76              |
| 30:D5:25:LEU:HD12  | 55:DW:19:LEU:HB3   | 1.67                     | 0.76              |
| 1:AA:309:G:H1'     | 1:AA:608:A:C2      | 2.21                     | 0.76              |
| 24:AY:238:THR:HG22 | 24:AY:241:GLU:CG   | 2.16                     | 0.76              |
| 27:B2:69:ARG:NH2   | 35:BA:111:A:H4'    | 2.00                     | 0.76              |
| 35:BA:2636:U:H4'   | 39:BE:80:GLU:OE1   | 1.86                     | 0.76              |
| 35:BA:2852:G:H2'   | 35:BA:2853:C:C6    | 2.20                     | 0.76              |
| 35:BA:882:G:H2'    | 35:BA:883:G:C8     | 2.20                     | 0.76              |
| 38:BD:144:ALA:HB3  | 38:BD:192:THR:HG23 | 1.66                     | 0.76              |
| 46:BN:57:ALA:H     | 46:BN:124:ALA:HA   | 1.50                     | 0.76              |
| 53:BU:92:ARG:O     | 53:BU:94:ASN:N     | 2.18                     | 0.76              |
| 54:BV:58:VAL:O     | 54:BV:97:LYS:HB2   | 1.85                     | 0.76              |
| 57:BY:8:LYS:HD2    | 57:BY:8:LYS:N      | 2.01                     | 0.76              |
| 1:CA:1239:A:H2'    | 1:CA:1298:C:H42    | 1.50                     | 0.76              |
| 27:D2:10:LEU:O     | 27:D2:14:ARG:HG2   | 1.86                     | 0.76              |
| 41:DG:67:LYS:HD3   | 41:DG:68:PRO:N     | 2.00                     | 0.76              |
| 51:DS:96:GLY:O     | 51:DS:98:VAL:N     | 2.18                     | 0.76              |
| 10:AJ:54:PHE:CG    | 10:AJ:55:LYS:HE3   | 2.20                     | 0.76              |
| 10:AJ:71:LEU:HD12  | 10:AJ:72:VAL:H     | 1.51                     | 0.76              |
| 10:AJ:3:LYS:HZ2    | 10:AJ:76:ASN:HA    | 1.51                     | 0.76              |
| 27:B2:69:ARG:CG    | 27:B2:70:GLN:H     | 1.99                     | 0.76              |
| 35:BA:676:A:H1'    | 35:BA:2443:C:H1'   | 1.68                     | 0.76              |
| 41:BG:106:LEU:HA   | 41:BG:110:ALA:HB3  | 1.66                     | 0.76              |
| 50:BR:87:TYR:O     | 50:BR:89:ASP:N     | 2.19                     | 0.76              |
| 3:CC:175:LEU:HD21  | 3:CC:201:TYR:CE2   | 2.20                     | 0.76              |
| 9:CI:95:LYS:HD3    | 9:CI:96:LEU:N      | 2.00                     | 0.76              |
| 28:D3:8:LEU:HD22   | 28:D3:31:LEU:CD2   | 2.14                     | 0.76              |
| 31:D6:11:LEU:HG    | 31:D6:26:ASN:HD21  | 1.51                     | 0.76              |
| 35:DA:142:A:H8     | 35:DA:1595:G:H21   | 1.32                     | 0.76              |
| 35:DA:556:G:H2'    | 35:DA:557:U:C6     | 2.21                     | 0.76              |
| 36:DB:112:U:H2'    | 36:DB:113:G:H8     | 1.49                     | 0.76              |
| 35:DA:674:G:H1'    | 40:DF:74:ARG:HD3   | 1.68                     | 0.76              |
| 33:D8:13:ARG:HD3   | 48:DP:61:ARG:O     | 1.86                     | 0.76              |
| 52:DT:115:ARG:HB3  | 52:DT:115:ARG:NH1  | 2.01                     | 0.76              |
| 11:AK:58:PRO:HA    | 11:AK:90:GLY:HA3   | 1.68                     | 0.75              |
| 35:BA:286:C:H6     | 35:BA:286:C:H5'    | 1.51                     | 0.75              |
| 54:BV:15:GLU:HB3   | 54:BV:16:PRO:CD    | 2.16                     | 0.75              |
| 55:BW:29:LEU:HD11  | 55:BW:51:LEU:HD11  | 1.67                     | 0.75              |
| 1:CA:1206:G:H4'    | 3:CC:192:THR:O     | 1.86                     | 0.75              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:CO:39:LEU:HD13  | 15:CO:56:LEU:HB2   | 1.68                     | 0.75              |
| 24:CY:227:ILE:HG23 | 24:CY:237:PRO:HG2  | 1.67                     | 0.75              |
| 35:DA:2262:U:H2'   | 35:DA:2263:C:C5'   | 2.16                     | 0.75              |
| 35:DA:979:G:H3'    | 35:DA:980:A:H5'    | 1.68                     | 0.75              |
| 39:DE:200:GLU:N    | 39:DE:200:GLU:OE2  | 2.17                     | 0.75              |
| 48:DP:95:VAL:HA    | 48:DP:99:LEU:HD23  | 1.67                     | 0.75              |
| 53:DU:54:LYS:O     | 53:DU:58:ARG:HG3   | 1.86                     | 0.75              |
| 5:AE:87:SER:HB3    | 5:AE:131:ILE:CD1   | 2.16                     | 0.75              |
| 10:AJ:96:ILE:HD13  | 10:AJ:96:ILE:H     | 1.50                     | 0.75              |
| 24:AY:6:GLU:HG2    | 24:AY:6:GLU:O      | 1.86                     | 0.75              |
| 35:BA:840:C:H2'    | 35:BA:841:A:H5''   | 1.69                     | 0.75              |
| 35:BA:878:A:H2'    | 35:BA:879:G:O4'    | 1.87                     | 0.75              |
| 38:BD:261:LYS:NZ   | 38:BD:263:ARG:HH12 | 1.85                     | 0.75              |
| 41:BG:172:LEU:CD2  | 41:BG:176:LEU:HD11 | 2.16                     | 0.75              |
| 41:BG:97:ASP:HB2   | 41:BG:98:ARG:NH1   | 2.00                     | 0.75              |
| 42:BH:149:ARG:HD3  | 42:BH:164:TYR:CE1  | 2.21                     | 0.75              |
| 49:BQ:6:ARG:O      | 49:BQ:7:MET:HG3    | 1.84                     | 0.75              |
| 10:CJ:40:LEU:HD23  | 10:CJ:40:LEU:N     | 2.01                     | 0.75              |
| 24:CY:137:ASN:HD21 | 24:CY:263:ALA:HB3  | 1.50                     | 0.75              |
| 24:CY:289:ILE:HG22 | 24:CY:290:LYS:N    | 2.01                     | 0.75              |
| 27:D2:6:VAL:HA     | 27:D2:9:GLN:OE1    | 1.86                     | 0.75              |
| 33:D8:56:GLU:HA    | 33:D8:59:LYS:HZ1   | 1.48                     | 0.75              |
| 34:D9:27:CYS:SG    | 34:D9:28:GLU:N     | 2.60                     | 0.75              |
| 41:DG:107:LEU:HD11 | 41:DG:178:PHE:CE1  | 2.21                     | 0.75              |
| 46:DN:23:LEU:HB3   | 46:DN:60:ILE:HG21  | 1.68                     | 0.75              |
| 51:DS:13:ARG:CG    | 51:DS:14:VAL:H     | 1.93                     | 0.75              |
| 52:DT:28:VAL:CG2   | 52:DT:46:GLU:HA    | 2.15                     | 0.75              |
| 57:DY:8:LYS:HB2    | 57:DY:28:LYS:HZ1   | 1.51                     | 0.75              |
| 4:AD:61:LYS:HE2    | 4:AD:62:GLN:HE21   | 1.52                     | 0.75              |
| 24:AY:281:PRO:HB2  | 24:AY:286:ILE:CD1  | 2.15                     | 0.75              |
| 24:AY:363:ARG:HH11 | 24:AY:363:ARG:HG3  | 1.51                     | 0.75              |
| 26:B1:3:LYS:HG3    | 26:B1:4:VAL:H      | 1.51                     | 0.75              |
| 35:BA:1748:G:H8    | 35:BA:1748:G:H5'   | 1.51                     | 0.75              |
| 35:BA:991:C:H6     | 35:BA:991:C:H5'    | 1.50                     | 0.75              |
| 44:BK:17:ALA:HB3   | 44:BK:38:VAL:HG22  | 1.67                     | 0.75              |
| 48:BP:95:VAL:HA    | 48:BP:99:LEU:HD23  | 1.68                     | 0.75              |
| 52:BT:129:ARG:NH2  | 52:BT:130:ALA:HA   | 2.01                     | 0.75              |
| 2:CB:124:SER:OG    | 2:CB:125:PRO:HD2   | 1.85                     | 0.75              |
| 13:CM:66:LEU:HD12  | 13:CM:66:LEU:N     | 2.00                     | 0.75              |
| 19:CS:14:HIS:HD2   | 19:CS:15:LEU:HD23  | 1.50                     | 0.75              |
| 22:CW:41:C:O2'     | 22:CW:42:C:H5'     | 1.86                     | 0.75              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:D4:13:ARG:HH11  | 29:D4:13:ARG:HB3   | 1.50                     | 0.75              |
| 34:D9:18:ARG:O     | 34:D9:18:ARG:HG2   | 1.86                     | 0.75              |
| 35:DA:2789:C:H1'   | 35:DA:2892:A:C2    | 2.21                     | 0.75              |
| 35:DA:840:C:H2'    | 35:DA:841:A:H5''   | 1.68                     | 0.75              |
| 40:DF:157:VAL:CG2  | 40:DF:194:MET:HG2  | 2.16                     | 0.75              |
| 41:DG:39:ILE:HA    | 41:DG:156:ASP:O    | 1.86                     | 0.75              |
| 54:DV:45:THR:O     | 54:DV:46:VAL:HG12  | 1.85                     | 0.75              |
| 3:AC:86:VAL:O      | 3:AC:89:GLU:HB3    | 1.85                     | 0.75              |
| 16:AP:25:ARG:HH11  | 16:AP:25:ARG:HG3   | 1.51                     | 0.75              |
| 31:B6:5:VAL:HG12   | 31:B6:6:ARG:O      | 1.86                     | 0.75              |
| 39:BE:200:GLU:OE2  | 39:BE:200:GLU:N    | 2.18                     | 0.75              |
| 39:BE:50:GLY:HA2   | 39:BE:78:LEU:HB3   | 1.68                     | 0.75              |
| 42:BH:175:LYS:O    | 42:BH:176:ALA:CB   | 2.33                     | 0.75              |
| 46:BN:67:LEU:O     | 46:BN:68:GLU:HB2   | 1.86                     | 0.75              |
| 19:CS:78:ARG:HB2   | 19:CS:81:ARG:HH11  | 1.51                     | 0.75              |
| 24:CY:491:VAL:HG13 | 24:CY:596:LYS:HE2  | 1.67                     | 0.75              |
| 35:DA:2020:A:C2'   | 35:DA:2021:C:H5''  | 2.17                     | 0.75              |
| 35:DA:2461:C:H5'   | 35:DA:2462:U:OP2   | 1.85                     | 0.75              |
| 42:DH:13:LYS:HA    | 42:DH:13:LYS:HE2   | 1.67                     | 0.75              |
| 52:DT:89:VAL:HG12  | 52:DT:91:ARG:HG3   | 1.68                     | 0.75              |
| 53:DU:47:TYR:HA    | 53:DU:50:ARG:HH21  | 1.51                     | 0.75              |
| 53:DU:112:ARG:HH22 | 54:DV:46:VAL:HG11  | 1.49                     | 0.75              |
| 56:DX:35:THR:O     | 56:DX:39:ILE:HG12  | 1.86                     | 0.75              |
| 10:AJ:63:PHE:HB3   | 14:AN:58:LYS:HA    | 1.66                     | 0.75              |
| 13:AM:6:GLY:C      | 13:AM:8:GLU:H      | 1.90                     | 0.75              |
| 14:AN:27:CYS:HG    | 59:AN:101:ZN:ZN    | 0.95                     | 0.75              |
| 35:BA:2147:G:H2'   | 35:BA:2148:G:O4'   | 1.85                     | 0.75              |
| 36:BB:87:G:H3'     | 36:BB:88:C:H5''    | 1.68                     | 0.75              |
| 38:BD:132:PRO:HG3  | 38:BD:190:TYR:CE1  | 2.22                     | 0.75              |
| 42:BH:66:GLY:HA2   | 42:BH:69:ARG:HB3   | 1.68                     | 0.75              |
| 56:BX:35:THR:O     | 56:BX:39:ILE:HG12  | 1.87                     | 0.75              |
| 1:CA:1030(D):A:H2' | 1:CA:1031:G:H5'    | 1.68                     | 0.75              |
| 10:CJ:63:PHE:HB3   | 14:CN:58:LYS:HA    | 1.68                     | 0.75              |
| 24:CY:16:GLY:O     | 24:CY:104:ALA:HB1  | 1.86                     | 0.75              |
| 35:DA:676:A:H8     | 35:DA:2069:G:H21   | 1.32                     | 0.75              |
| 35:DA:2178:C:H4'   | 37:DC:47:LYS:HD3   | 1.68                     | 0.75              |
| 38:DD:44:ASN:HB2   | 38:DD:48:ARG:O     | 1.85                     | 0.75              |
| 54:DV:77:ALA:O     | 54:DV:79:VAL:HG23  | 1.87                     | 0.75              |
| 58:DZ:182:LYS:O    | 58:DZ:183:LEU:HD23 | 1.86                     | 0.75              |
| 1:AA:1014:A:H4'    | 19:AS:14:HIS:CE1   | 2.22                     | 0.75              |
| 2:AB:165:VAL:HG23  | 2:AB:166:ASP:N     | 2.01                     | 0.75              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:AE:81:GLU:HG2    | 5:AE:90:VAL:HG22   | 1.68                     | 0.75              |
| 16:AP:74:LEU:HD23  | 16:AP:79:VAL:HG21  | 1.68                     | 0.75              |
| 30:B5:4:HIS:CB     | 30:B5:5:PRO:HD3    | 2.16                     | 0.75              |
| 35:BA:1946:U:H2'   | 35:BA:1947:C:C6    | 2.22                     | 0.75              |
| 35:BA:2593:U:H2'   | 35:BA:2594:C:H6    | 1.52                     | 0.75              |
| 35:BA:2666:C:H5'   | 35:BA:2667:C:OP2   | 1.87                     | 0.75              |
| 35:BA:279:C:H2'    | 35:BA:280:C:H5''   | 1.68                     | 0.75              |
| 1:CA:559:A:H4'     | 1:CA:560:U:H5'     | 1.68                     | 0.75              |
| 35:DA:286:C:H6     | 35:DA:286:C:H5'    | 1.52                     | 0.75              |
| 35:DA:83:G:O2'     | 35:DA:84:A:H8      | 1.68                     | 0.75              |
| 22:AV:53:G:O2'     | 22:AV:54:5MU:H5''  | 1.86                     | 0.75              |
| 24:AY:453:GLY:HA3  | 24:AY:459:LEU:CD1  | 2.16                     | 0.75              |
| 35:BA:1963:U:H2'   | 35:BA:1963:U:O2    | 1.86                     | 0.75              |
| 35:BA:676:A:H8     | 35:BA:2069:G:H21   | 1.33                     | 0.75              |
| 35:BA:2308:G:O6    | 35:BA:2310:A:H2'   | 1.87                     | 0.75              |
| 36:BB:48:A:H4'     | 51:BS:95:HIS:HD2   | 1.50                     | 0.75              |
| 46:BN:65:LYS:HB3   | 46:BN:69:GLN:HG3   | 1.68                     | 0.75              |
| 48:BP:126:VAL:HA   | 48:BP:145:PRO:CB   | 2.16                     | 0.75              |
| 52:BT:118:ARG:HA   | 52:BT:121:ILE:HB   | 1.67                     | 0.75              |
| 52:BT:89:VAL:HG12  | 52:BT:91:ARG:HG3   | 1.67                     | 0.75              |
| 1:CA:625:G:H2'     | 1:CA:626:U:C6      | 2.21                     | 0.75              |
| 2:CB:17:PHE:HB3    | 2:CB:44:LEU:HD21   | 1.68                     | 0.75              |
| 24:CY:517:LEU:HD11 | 24:CY:564:LYS:HB2  | 1.68                     | 0.75              |
| 26:D1:92:LYS:HE2   | 35:DA:153:C:OP1    | 1.87                     | 0.75              |
| 7:AG:145:ALA:O     | 7:AG:146:GLU:HB2   | 1.85                     | 0.75              |
| 18:AR:31:LEU:H     | 18:AR:31:LEU:HD23  | 1.51                     | 0.75              |
| 19:AS:14:HIS:HD2   | 19:AS:15:LEU:HD23  | 1.52                     | 0.75              |
| 19:AS:44:MET:SD    | 19:AS:44:MET:N     | 2.59                     | 0.75              |
| 24:AY:215:LYS:O    | 24:AY:219:VAL:HG23 | 1.86                     | 0.75              |
| 39:BE:59:VAL:HG11  | 39:BE:63:LEU:HG    | 1.68                     | 0.75              |
| 41:BG:145:THR:HG23 | 41:BG:148:MET:HB2  | 1.66                     | 0.75              |
| 42:BH:18:GLU:HB2   | 42:BH:25:LYS:HB2   | 1.67                     | 0.75              |
| 58:BZ:166:SER:HB2  | 58:BZ:167:PRO:CA   | 2.17                     | 0.75              |
| 1:CA:178:C:O2'     | 1:CA:179:A:H5'     | 1.85                     | 0.75              |
| 3:CC:16:ARG:HH11   | 3:CC:16:ARG:CB     | 2.00                     | 0.75              |
| 24:CY:170:ARG:HD2  | 24:CY:170:ARG:N    | 2.00                     | 0.75              |
| 35:DA:2666:C:H5'   | 35:DA:2667:C:OP2   | 1.86                     | 0.75              |
| 35:DA:395:U:H2'    | 35:DA:396:G:C8     | 2.20                     | 0.75              |
| 38:DD:132:PRO:HG3  | 38:DD:190:TYR:CE1  | 2.21                     | 0.75              |
| 40:DF:28:ILE:HD13  | 40:DF:28:ILE:H     | 1.49                     | 0.75              |
| 41:DG:111:LEU:HB2  | 41:DG:112:PRO:HD3  | 1.68                     | 0.75              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:DK:17:ALA:CB    | 44:DK:38:VAL:HG22  | 2.17                     | 0.75              |
| 50:DR:87:TYR:O     | 50:DR:89:ASP:N     | 2.19                     | 0.75              |
| 1:AA:1206:G:H4'    | 3:AC:192:THR:O     | 1.87                     | 0.75              |
| 12:AL:45:PRO:HG3   | 12:AL:53:ARG:HD3   | 1.69                     | 0.75              |
| 24:AY:313:ALA:HA   | 24:AY:328:ILE:HG22 | 1.67                     | 0.75              |
| 36:BB:86:G:H2'     | 36:BB:87:G:C8      | 2.21                     | 0.75              |
| 37:BC:28:ARG:HG2   | 37:BC:183:PRO:HB3  | 1.68                     | 0.75              |
| 6:CF:45:LEU:O      | 6:CF:46:ARG:HG3    | 1.87                     | 0.75              |
| 14:CN:41:ARG:HH11  | 14:CN:41:ARG:HG2   | 1.52                     | 0.75              |
| 24:CY:149:VAL:O    | 24:CY:152:THR:HG22 | 1.87                     | 0.75              |
| 26:D1:7:ILE:HG22   | 26:D1:66:HIS:HD2   | 1.49                     | 0.75              |
| 32:D7:23:ARG:C     | 32:D7:28:ARG:HH12  | 1.89                     | 0.75              |
| 35:DA:2852:G:H2'   | 35:DA:2853:C:C6    | 2.22                     | 0.75              |
| 36:DB:86:G:H2'     | 36:DB:87:G:C8      | 2.22                     | 0.75              |
| 46:DN:67:LEU:O     | 46:DN:68:GLU:HB2   | 1.85                     | 0.75              |
| 48:DP:126:VAL:HA   | 48:DP:145:PRO:CB   | 2.16                     | 0.75              |
| 1:AA:382:A:H2'     | 1:AA:383:A:C8      | 2.22                     | 0.74              |
| 4:AD:160:GLN:O     | 4:AD:163:GLU:HB3   | 1.87                     | 0.74              |
| 12:AL:80:HIS:O     | 12:AL:81:SER:HB2   | 1.86                     | 0.74              |
| 16:AP:22:THR:HA    | 16:AP:33:ILE:HG12  | 1.69                     | 0.74              |
| 34:B9:27:CYS:SG    | 34:B9:28:GLU:N     | 2.60                     | 0.74              |
| 32:B7:19:ARG:HD3   | 35:BA:125:G:H5'    | 1.69                     | 0.74              |
| 35:BA:654(G):C:H2' | 35:BA:654(H):G:H8  | 1.51                     | 0.74              |
| 38:BD:35:LYS:CG    | 38:BD:63:ARG:HG3   | 2.17                     | 0.74              |
| 41:BG:98:ARG:NH1   | 41:BG:98:ARG:HG2   | 2.01                     | 0.74              |
| 48:BP:16:ARG:HB2   | 48:BP:16:ARG:NH1   | 2.02                     | 0.74              |
| 50:BR:11:ASN:OD1   | 50:BR:12:ARG:N     | 2.20                     | 0.74              |
| 57:BY:62:GLU:HG2   | 57:BY:63:LYS:H     | 1.52                     | 0.74              |
| 1:CA:1321:C:C3'    | 1:CA:1322:C:H5''   | 2.16                     | 0.74              |
| 12:CL:27:LEU:O     | 12:CL:29:GLY:N     | 2.20                     | 0.74              |
| 24:CY:21:ILE:O     | 24:CY:22:ASP:HB2   | 1.84                     | 0.74              |
| 24:CY:486:THR:O    | 24:CY:600:VAL:HG12 | 1.87                     | 0.74              |
| 61:CY:702:FUA:C5   | 61:CY:702:FUA:H202 | 2.14                     | 0.74              |
| 22:CV:2:G:C5'      | 25:D0:8:GLY:HA2    | 2.17                     | 0.74              |
| 31:D6:35:GLU:CB    | 31:D6:51:GLU:HB2   | 2.17                     | 0.74              |
| 35:DA:108:U:H2'    | 35:DA:109:G:H8     | 1.50                     | 0.74              |
| 35:DA:2195:C:O2'   | 35:DA:2196:C:H5'   | 1.87                     | 0.74              |
| 35:DA:548:A:H2'    | 35:DA:549:G:H5'    | 1.67                     | 0.74              |
| 37:DC:23:ILE:HB    | 37:DC:229:SER:OXT  | 1.87                     | 0.74              |
| 48:DP:7:ARG:O      | 48:DP:10:PRO:HD2   | 1.86                     | 0.74              |
| 1:AA:1296:C:H5'    | 1:AA:1297:C:OP2    | 1.87                     | 0.74              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1369:C:H2'    | 1:AA:1370:G:C8     | 2.21                     | 0.74              |
| 2:AB:168:THR:HG23  | 2:AB:192:SER:CB    | 2.16                     | 0.74              |
| 24:AY:428:LEU:CD1  | 24:AY:440:VAL:HG11 | 2.17                     | 0.74              |
| 35:BA:751:A:H5'    | 55:BW:90:ARG:HA    | 1.69                     | 0.74              |
| 37:BC:23:ILE:HB    | 37:BC:229:SER:OXT  | 1.86                     | 0.74              |
| 39:BE:49:LEU:HD22  | 39:BE:49:LEU:N     | 2.01                     | 0.74              |
| 41:BG:60:LEU:O     | 41:BG:63:ILE:HD11  | 1.86                     | 0.74              |
| 47:BO:17:ARG:NE    | 47:BO:47:ILE:HD11  | 2.02                     | 0.74              |
| 35:BA:2392:A:H8    | 48:BP:60:MET:HB3   | 1.50                     | 0.74              |
| 1:CA:1072:G:H2'    | 1:CA:1073:U:C6     | 2.22                     | 0.74              |
| 10:CJ:47:PHE:CZ    | 14:CN:37:PHE:HE2   | 2.05                     | 0.74              |
| 19:CS:32:LYS:HA    | 19:CS:50:ALA:HB3   | 1.68                     | 0.74              |
| 24:CY:33:LEU:HD23  | 24:CY:360:ALA:CB   | 2.16                     | 0.74              |
| 24:CY:546:ILE:CD1  | 24:CY:565:VAL:HG11 | 2.17                     | 0.74              |
| 35:DA:2122:U:H2'   | 35:DA:2123:G:H8    | 1.51                     | 0.74              |
| 35:DA:297:C:H2'    | 35:DA:298:G:O4'    | 1.87                     | 0.74              |
| 35:DA:49:A:H5''    | 35:DA:51:G:O4'     | 1.88                     | 0.74              |
| 42:DH:20:ALA:HB1   | 42:DH:21:PRO:CD    | 2.17                     | 0.74              |
| 46:DN:58:ASP:C     | 46:DN:60:ILE:H     | 1.91                     | 0.74              |
| 50:DR:62:ALA:O     | 50:DR:66:VAL:HG23  | 1.87                     | 0.74              |
| 53:DU:110:VAL:HG12 | 53:DU:114:LYS:CD   | 2.17                     | 0.74              |
| 12:AL:41:ARG:CG    | 12:AL:42:THR:H     | 1.98                     | 0.74              |
| 61:AY:702:FUA:H202 | 61:AY:702:FUA:C5   | 2.15                     | 0.74              |
| 33:B8:2:PRO:HA     | 35:BA:591:C:O2     | 1.86                     | 0.74              |
| 40:BF:195:ASP:OD1  | 40:BF:196:LEU:N    | 2.18                     | 0.74              |
| 51:BS:34:HIS:CE1   | 51:BS:54:LEU:HB3   | 2.22                     | 0.74              |
| 53:BU:112:ARG:HH22 | 54:BV:46:VAL:HG11  | 1.52                     | 0.74              |
| 53:BU:54:LYS:O     | 53:BU:58:ARG:HG3   | 1.86                     | 0.74              |
| 56:BX:27:THR:HB    | 56:BX:80:ILE:HG22  | 1.68                     | 0.74              |
| 57:BY:8:LYS:HB2    | 57:BY:28:LYS:HZ3   | 1.50                     | 0.74              |
| 3:CC:86:VAL:O      | 3:CC:89:GLU:HB3    | 1.88                     | 0.74              |
| 24:CY:25:LYS:HE2   | 24:CY:86:GLY:H     | 1.52                     | 0.74              |
| 35:DA:1748:G:H8    | 35:DA:1748:G:H5'   | 1.51                     | 0.74              |
| 27:D2:47:ASN:ND2   | 35:DA:94(A):G:H21  | 1.85                     | 0.74              |
| 30:D5:55:ARG:HH22  | 50:DR:33:ARG:HG2   | 1.53                     | 0.74              |
| 16:AP:20:VAL:CG2   | 16:AP:32:TYR:HB2   | 2.15                     | 0.74              |
| 24:AY:423:LYS:HB3  | 24:AY:472:VAL:CG2  | 2.17                     | 0.74              |
| 24:AY:446:THR:O    | 24:AY:448:GLN:HG2  | 1.87                     | 0.74              |
| 35:BA:1220:A:H3'   | 35:BA:1221:C:H5'   | 1.69                     | 0.74              |
| 35:BA:548:A:H2'    | 35:BA:549:G:H5'    | 1.67                     | 0.74              |
| 35:BA:83:G:O2'     | 35:BA:84:A:H8      | 1.69                     | 0.74              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:BG:108:ASN:O    | 41:BG:109:VAL:HG23 | 1.87                     | 0.74              |
| 1:CA:235:C:H5'     | 17:CQ:70:ARG:HG2   | 1.70                     | 0.74              |
| 7:CG:145:ALA:O     | 7:CG:146:GLU:HB2   | 1.87                     | 0.74              |
| 18:CR:31:LEU:HD23  | 18:CR:31:LEU:H     | 1.51                     | 0.74              |
| 24:CY:529:ILE:HD11 | 24:CY:567:LEU:HD11 | 1.68                     | 0.74              |
| 35:DA:2150:U:H2'   | 35:DA:2151:G:C8    | 2.23                     | 0.74              |
| 35:DA:676:A:H1'    | 35:DA:2443:C:H1'   | 1.68                     | 0.74              |
| 35:DA:878:A:H2'    | 35:DA:879:G:O4'    | 1.87                     | 0.74              |
| 42:DH:96:ALA:HB1   | 42:DH:103:LEU:HD11 | 1.68                     | 0.74              |
| 48:DP:47:ASP:HB3   | 48:DP:48:PRO:HA    | 1.69                     | 0.74              |
| 50:DR:9:LYS:O      | 50:DR:10:LEU:HD23  | 1.85                     | 0.74              |
| 54:DV:18:LEU:CD2   | 54:DV:19:LYS:H     | 2.00                     | 0.74              |
| 58:DZ:29:TYR:HB3   | 58:DZ:34:ASN:CB    | 2.16                     | 0.74              |
| 1:AA:294:U:H2'     | 1:AA:295:C:H6      | 1.52                     | 0.74              |
| 1:AA:552:U:H4'     | 12:AL:86:ARG:HG2   | 1.69                     | 0.74              |
| 9:AI:47:LEU:N      | 9:AI:47:LEU:HD12   | 2.03                     | 0.74              |
| 10:AJ:82:ILE:O     | 10:AJ:86:MET:HB2   | 1.87                     | 0.74              |
| 20:AT:50:GLU:HG3   | 20:AT:51:GLU:N     | 2.01                     | 0.74              |
| 24:AY:165:GLN:HB2  | 24:AY:260:LEU:HD11 | 1.69                     | 0.74              |
| 24:AY:25:LYS:HE3   | 62:AY:703:GDP:PB   | 2.27                     | 0.74              |
| 35:BA:2020:A:O2'   | 35:BA:2021:C:H5''  | 1.87                     | 0.74              |
| 36:BB:7:G:C2'      | 36:BB:8:U:H5''     | 2.16                     | 0.74              |
| 18:CR:59:SER:H     | 18:CR:62:GLU:HB2   | 1.53                     | 0.74              |
| 26:D1:67:ILE:N     | 26:D1:68:PRO:HD2   | 2.02                     | 0.74              |
| 31:D6:6:ARG:N      | 31:D6:6:ARG:HD2    | 2.02                     | 0.74              |
| 35:DA:1001:A:H2'   | 35:DA:1002:G:O4'   | 1.87                     | 0.74              |
| 35:DA:2593:U:H2'   | 35:DA:2594:C:H6    | 1.51                     | 0.74              |
| 42:DH:17:VAL:O     | 42:DH:45:VAL:HG22  | 1.87                     | 0.74              |
| 42:DH:85:LYS:HZ3   | 42:DH:87:LEU:HG    | 1.53                     | 0.74              |
| 35:DA:84:A:H5''    | 57:DY:9:LYS:NZ     | 2.02                     | 0.74              |
| 1:AA:1321:C:C3'    | 1:AA:1322:C:H5''   | 2.17                     | 0.74              |
| 1:AA:179:A:H2'     | 1:AA:180:U:C6      | 2.22                     | 0.74              |
| 4:AD:98:GLU:HG2    | 4:AD:189:PRO:HG3   | 1.69                     | 0.74              |
| 8:AH:17:THR:HB     | 8:AH:78:GLN:OE1    | 1.87                     | 0.74              |
| 14:AN:23:ARG:HD2   | 14:AN:28:GLY:O     | 1.86                     | 0.74              |
| 1:AA:275:G:H5''    | 17:AQ:14:LYS:HB2   | 1.68                     | 0.74              |
| 17:AQ:67:LYS:HA    | 17:AQ:70:ARG:HH12  | 1.53                     | 0.74              |
| 19:AS:9:VAL:O      | 19:AS:11:VAL:N     | 2.21                     | 0.74              |
| 35:BA:2713:A:H3'   | 35:BA:2714:G:H5'   | 1.69                     | 0.74              |
| 1:CA:1116:C:H2'    | 1:CA:1117:G:H5''   | 1.70                     | 0.74              |
| 5:CE:9:LYS:CB      | 5:CE:112:LEU:HD11  | 2.18                     | 0.74              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:DA:1220:A:H3'   | 35:DA:1221:C:H5'  | 1.68                     | 0.74              |
| 36:DB:87:G:H3'     | 36:DB:88:C:H5''   | 1.69                     | 0.74              |
| 58:DZ:97:GLU:HG3   | 58:DZ:127:LYS:HD3 | 1.70                     | 0.74              |
| 24:AY:225:GLU:HB2  | 24:AY:228:MET:HE1 | 1.69                     | 0.74              |
| 23:AX:19:U:H5''    | 24:AY:504:ARG:HD3 | 1.68                     | 0.74              |
| 34:B9:18:ARG:O     | 34:B9:18:ARG:HG2  | 1.87                     | 0.74              |
| 35:BA:2461:C:H5'   | 35:BA:2462:U:OP2  | 1.87                     | 0.74              |
| 51:BS:95:HIS:CG    | 51:BS:96:GLY:H    | 2.06                     | 0.74              |
| 3:CC:58:GLU:O      | 3:CC:59:ARG:HG3   | 1.87                     | 0.74              |
| 4:CD:61:LYS:HE2    | 4:CD:62:GLN:HE21  | 1.52                     | 0.74              |
| 5:CE:76:ILE:HG13   | 5:CE:142:LEU:HD13 | 1.70                     | 0.74              |
| 28:D3:56:VAL:HG12  | 28:D3:57:GLU:H    | 1.52                     | 0.74              |
| 32:D7:24:THR:HG23  | 32:D7:27:GLY:H    | 1.53                     | 0.74              |
| 35:DA:2132:U:C4    | 37:DC:6:LYS:HD2   | 2.23                     | 0.74              |
| 35:DA:2313:C:H5'   | 35:DA:2313:C:H6   | 1.53                     | 0.74              |
| 35:DA:580:C:H2'    | 35:DA:581:C:H6    | 1.53                     | 0.74              |
| 39:DE:11:MET:HB2   | 39:DE:23:VAL:O    | 1.88                     | 0.74              |
| 3:AC:58:GLU:O      | 3:AC:59:ARG:HG3   | 1.86                     | 0.74              |
| 35:BA:1996:C:H4'   | 35:BA:1997:G:H5'  | 1.68                     | 0.74              |
| 42:BH:171:LEU:CD2  | 42:BH:172:LYS:O   | 2.35                     | 0.74              |
| 48:BP:97:PRO:O     | 48:BP:98:GLU:HB3  | 1.88                     | 0.74              |
| 6:CF:37:VAL:HG12   | 6:CF:38:GLU:N     | 2.01                     | 0.74              |
| 16:CP:53:VAL:HG23  | 16:CP:54:GLU:H    | 1.53                     | 0.74              |
| 24:CY:454:MET:H    | 24:CY:458:HIS:CD2 | 2.04                     | 0.74              |
| 35:DA:279:C:H2'    | 35:DA:280:C:H5''  | 1.70                     | 0.74              |
| 44:DK:57:ILE:HD12  | 44:DK:57:ILE:H    | 1.52                     | 0.74              |
| 1:AA:1004:A:N6     | 1:AA:1034:G:H2'   | 2.02                     | 0.74              |
| 1:AA:939:G:H5''    | 7:AG:102:ARG:HH22 | 1.52                     | 0.74              |
| 27:B2:69:ARG:HG3   | 27:B2:70:GLN:N    | 2.03                     | 0.74              |
| 30:B5:58:LEU:O     | 30:B5:58:LEU:HD22 | 1.88                     | 0.74              |
| 31:B6:27:LYS:O     | 31:B6:27:LYS:HD2  | 1.87                     | 0.74              |
| 35:BA:2645:G:C3'   | 35:BA:2646:C:H5'  | 2.13                     | 0.74              |
| 53:BU:110:VAL:HG12 | 53:BU:114:LYS:CD  | 2.18                     | 0.74              |
| 1:CA:382:A:H2'     | 1:CA:383:A:C8     | 2.23                     | 0.74              |
| 10:CJ:48:THR:HG23  | 10:CJ:62:HIS:ND1  | 2.03                     | 0.74              |
| 26:D1:76:ARG:NH2   | 26:D1:95:LEU:HD13 | 2.00                     | 0.74              |
| 35:DA:2147:G:H2'   | 35:DA:2148:G:O4'  | 1.88                     | 0.74              |
| 35:DA:745:G:H5'    | 35:DA:746:A:OP2   | 1.88                     | 0.74              |
| 56:DX:8:ILE:N      | 56:DX:8:ILE:HD12  | 2.03                     | 0.74              |
| 1:AA:953:G:H5'     | 1:AA:965:A:H61    | 1.53                     | 0.74              |
| 18:AR:59:SER:H     | 18:AR:62:GLU:HB2  | 1.52                     | 0.74              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 24:AY:512:ILE:HD12 | 24:AY:589:ALA:HB1   | 1.69                     | 0.74              |
| 31:B6:41:PRO:HD2   | 31:B6:45:LYS:O      | 1.88                     | 0.74              |
| 35:BA:2577:A:H5'   | 35:BA:2578:G:H5'    | 1.69                     | 0.74              |
| 35:BA:914:C:H2'    | 35:BA:915:C:H5'     | 1.69                     | 0.74              |
| 39:BE:36:ARG:HH21  | 39:BE:88:GLY:CA     | 2.00                     | 0.74              |
| 44:BK:42:ASN:O     | 44:BK:46:ALA:HB2    | 1.87                     | 0.74              |
| 52:BT:28:VAL:CG2   | 52:BT:46:GLU:HA     | 2.17                     | 0.74              |
| 54:BV:15:GLU:CB    | 54:BV:16:PRO:HD2    | 2.18                     | 0.74              |
| 1:CA:1239:A:H2'    | 1:CA:1298:C:N4      | 2.01                     | 0.74              |
| 1:CA:1342:C:O2'    | 1:CA:1343:G:H5'     | 1.88                     | 0.74              |
| 1:CA:939:G:H5''    | 7:CG:102:ARG:HH22   | 1.50                     | 0.74              |
| 3:CC:181:ASN:ND2   | 3:CC:204:LEU:HB2    | 2.03                     | 0.74              |
| 16:CP:21:VAL:O     | 16:CP:33:ILE:HB     | 1.88                     | 0.74              |
| 24:CY:673:PHE:CG   | 24:CY:674:ASP:N     | 2.55                     | 0.74              |
| 27:D2:4:SER:HA     | 27:D2:7:ARG:NH1     | 2.02                     | 0.74              |
| 35:DA:1053:C:H2'   | 35:DA:1054:A:H5''   | 1.69                     | 0.74              |
| 25:D0:60:PHE:HE2   | 35:DA:2365:G:H4'    | 1.50                     | 0.74              |
| 40:DF:65:TRP:HZ3   | 40:DF:75:HIS:HD2    | 1.35                     | 0.74              |
| 41:DG:46:ALA:CB    | 41:DG:88:ILE:HB     | 2.16                     | 0.74              |
| 44:DK:42:ASN:O     | 44:DK:46:ALA:HB2    | 1.88                     | 0.74              |
| 35:DA:2392:A:H8    | 48:DP:60:MET:HB3    | 1.52                     | 0.74              |
| 26:B1:45:ASN:HD22  | 26:B1:45:ASN:C      | 1.90                     | 0.73              |
| 35:BA:1434:A:H61   | 35:BA:1558:A:H62    | 1.31                     | 0.73              |
| 35:BA:419:C:H2'    | 35:BA:420:C:H6      | 1.53                     | 0.73              |
| 35:BA:580:C:H2'    | 35:BA:581:C:H6      | 1.53                     | 0.73              |
| 48:BP:62:LEU:CD2   | 48:BP:62:LEU:H      | 2.01                     | 0.73              |
| 2:CB:204:ASN:C     | 2:CB:204:ASN:HD22   | 1.91                     | 0.73              |
| 20:CT:50:GLU:HG3   | 20:CT:51:GLU:N      | 2.01                     | 0.73              |
| 34:D9:36:GLN:OE1   | 35:DA:1124:C:H1'    | 1.87                     | 0.73              |
| 38:DD:34:VAL:HG23  | 38:DD:35:LYS:N      | 2.03                     | 0.73              |
| 41:DG:42:GLY:HA2   | 41:DG:89:GLY:HA2    | 1.69                     | 0.73              |
| 48:DP:97:PRO:O     | 48:DP:98:GLU:HB3    | 1.88                     | 0.73              |
| 35:DA:2470:G:P     | 49:DQ:56:ARG:HH12   | 2.11                     | 0.73              |
| 58:DZ:102:LEU:HD21 | 58:DZ:124:ILE:CD1   | 2.18                     | 0.73              |
| 4:AD:4:TYR:O       | 4:AD:5:ILE:HB       | 1.86                     | 0.73              |
| 29:B4:8:LYS:O      | 29:B4:9:LEU:HB2     | 1.87                     | 0.73              |
| 31:B6:6:ARG:HD2    | 31:B6:6:ARG:N       | 2.03                     | 0.73              |
| 35:BA:2796:U:H3'   | 35:BA:2799:C:C5'    | 2.18                     | 0.73              |
| 35:BA:654(S):G:H3' | 35:BA:654(T):C:H5'' | 1.69                     | 0.73              |
| 38:BD:35:LYS:HD2   | 38:BD:35:LYS:C      | 2.09                     | 0.73              |
| 39:BE:47:VAL:HG12  | 39:BE:48:GLN:N      | 2.02                     | 0.73              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:BS:98:VAL:C    | 51:BS:100:ALA:H    | 1.92                     | 0.73              |
| 54:BV:46:VAL:HG22 | 54:BV:47:VAL:H     | 1.51                     | 0.73              |
| 1:CA:1117:G:O2'   | 9:CI:104:ARG:HD3   | 1.88                     | 0.73              |
| 10:CJ:48:THR:HA   | 10:CJ:62:HIS:CB    | 2.15                     | 0.73              |
| 38:DD:243:GLY:O   | 38:DD:244:ARG:HB3  | 1.88                     | 0.73              |
| 44:DK:93:ARG:HB2  | 58:DZ:112:ARG:NE   | 2.01                     | 0.73              |
| 58:DZ:12:GLY:HA2  | 58:DZ:36:LYS:NZ    | 2.03                     | 0.73              |
| 3:AC:175:LEU:HD21 | 3:AC:201:TYR:HE2   | 1.51                     | 0.73              |
| 24:AY:406:GLU:HB3 | 24:AY:407:PRO:HD2  | 1.71                     | 0.73              |
| 35:BA:1390:U:O2'  | 35:BA:1391:U:H5'   | 1.88                     | 0.73              |
| 35:BA:1948:G:C8   | 35:BA:1948:G:H5'   | 2.24                     | 0.73              |
| 35:BA:218:A:H2    | 35:BA:235:U:H4'    | 1.50                     | 0.73              |
| 41:BG:77:ILE:CG2  | 41:BG:80:PHE:H     | 1.90                     | 0.73              |
| 50:BR:62:ALA:O    | 50:BR:66:VAL:HG23  | 1.88                     | 0.73              |
| 30:B5:27:PRO:HG3  | 55:BW:23:LEU:HD11  | 1.70                     | 0.73              |
| 1:CA:1352:C:H2'   | 1:CA:1353:G:C8     | 2.23                     | 0.73              |
| 3:CC:46:GLU:O     | 3:CC:47:LEU:HB2    | 1.85                     | 0.73              |
| 27:D2:36:ARG:HA   | 27:D2:39:ALA:HB3   | 1.69                     | 0.73              |
| 31:D6:41:PRO:HD2  | 31:D6:45:LYS:O     | 1.87                     | 0.73              |
| 35:DA:1996:C:H4'  | 35:DA:1997:G:H5'   | 1.70                     | 0.73              |
| 48:DP:47:ASP:HB3  | 48:DP:48:PRO:CA    | 2.18                     | 0.73              |
| 49:DQ:21:THR:O    | 49:DQ:22:LYS:HB3   | 1.88                     | 0.73              |
| 5:AE:9:LYS:CB     | 5:AE:112:LEU:HD11  | 2.19                     | 0.73              |
| 11:AK:122:LYS:O   | 11:AK:124:LYS:N    | 2.22                     | 0.73              |
| 18:AR:29:PHE:CD2  | 18:AR:29:PHE:N     | 2.56                     | 0.73              |
| 22:AW:8:U:H3      | 22:AW:14:A:H62     | 1.33                     | 0.73              |
| 24:AY:128:TYR:O   | 24:AY:129:LYS:HB2  | 1.88                     | 0.73              |
| 35:BA:2146:C:H4'  | 35:BA:2147:G:C8    | 2.22                     | 0.73              |
| 36:BB:13:A:O2'    | 36:BB:14:U:H3'     | 1.87                     | 0.73              |
| 36:BB:3:C:N4      | 36:BB:118:G:H1     | 1.86                     | 0.73              |
| 52:BT:5:ALA:O     | 52:BT:7:ILE:N      | 2.21                     | 0.73              |
| 55:BW:78:GLU:OE2  | 55:BW:99:ARG:HD2   | 1.89                     | 0.73              |
| 56:BX:8:ILE:HD12  | 56:BX:8:ILE:N      | 2.02                     | 0.73              |
| 1:CA:792:A:O2'    | 1:CA:794:A:N7      | 2.20                     | 0.73              |
| 2:CB:83:MET:HG3   | 2:CB:234:PRO:HG3   | 1.69                     | 0.73              |
| 24:CY:102:ASP:O   | 24:CY:131:PRO:HD2  | 1.88                     | 0.73              |
| 24:CY:428:LEU:H   | 24:CY:428:LEU:HD23 | 1.54                     | 0.73              |
| 35:DA:288:C:H2'   | 35:DA:289:A:C8     | 2.24                     | 0.73              |
| 35:DA:662:G:OP1   | 48:DP:18:ARG:HD2   | 1.88                     | 0.73              |
| 38:DD:65:ILE:HG22 | 38:DD:104:TYR:CB   | 2.19                     | 0.73              |
| 41:DG:131:TYR:HE2 | 41:DG:133:LEU:HD23 | 1.52                     | 0.73              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:AA:447:G:H2'      | 1:AA:485:G:N2      | 2.03                     | 0.73              |
| 5:AE:51:VAL:HB      | 5:AE:52:PRO:HD3    | 1.69                     | 0.73              |
| 13:AM:78:ILE:HA     | 13:AM:81:LEU:HD23  | 1.71                     | 0.73              |
| 19:AS:22:LEU:O      | 19:AS:26:GLY:HA2   | 1.88                     | 0.73              |
| 25:B0:77:ARG:HH22   | 35:BA:857:C:H5'    | 1.53                     | 0.73              |
| 31:B6:15:GLU:OE2    | 31:B6:44:ARG:NH1   | 2.21                     | 0.73              |
| 35:BA:120:U:H2'     | 35:BA:120:U:O2     | 1.87                     | 0.73              |
| 35:BA:1689:A:H62    | 35:BA:1698:A:H2    | 1.33                     | 0.73              |
| 38:BD:176:ARG:HG2   | 38:BD:176:ARG:HH11 | 1.53                     | 0.73              |
| 41:BG:131:TYR:HB3   | 41:BG:159:VAL:HG13 | 1.71                     | 0.73              |
| 46:BN:26:LEU:HD12   | 46:BN:26:LEU:C     | 2.09                     | 0.73              |
| 46:BN:58:ASP:C      | 46:BN:60:ILE:H     | 1.92                     | 0.73              |
| 48:BP:47:ASP:HB3    | 48:BP:48:PRO:HA    | 1.70                     | 0.73              |
| 48:BP:58:THR:O      | 48:BP:61:ARG:NE    | 2.19                     | 0.73              |
| 49:BQ:29:PHE:HB2    | 49:BQ:105:GLU:OE2  | 1.89                     | 0.73              |
| 35:BA:2470:G:P      | 49:BQ:56:ARG:HH12  | 2.11                     | 0.73              |
| 30:B5:25:LEU:HD12   | 55:BW:19:LEU:HB3   | 1.70                     | 0.73              |
| 35:BA:64:A:C4       | 56:BX:66:LEU:HD13  | 2.24                     | 0.73              |
| 44:BK:93:ARG:HG3    | 58:BZ:112:ARG:HE   | 1.53                     | 0.73              |
| 1:CA:731:G:OP1      | 1:CA:766:A:H1'     | 1.88                     | 0.73              |
| 5:CE:98:THR:HB      | 5:CE:117:ASP:HB3   | 1.69                     | 0.73              |
| 24:CY:606:MET:O     | 24:CY:646:PHE:HA   | 1.89                     | 0.73              |
| 35:DA:1540:U:H3'    | 35:DA:1541:G:H3'   | 1.70                     | 0.73              |
| 35:DA:545:C:C3'     | 35:DA:547:A:H5"    | 2.19                     | 0.73              |
| 35:DA:654(M):C:HO2' | 35:DA:654(N):G:H8  | 1.36                     | 0.73              |
| 38:DD:172:TYR:HD1   | 38:DD:186:HIS:HA   | 1.52                     | 0.73              |
| 40:DF:139:PHE:HB2   | 40:DF:166:ALA:HB1  | 1.68                     | 0.73              |
| 50:DR:11:ASN:OD1    | 50:DR:12:ARG:N     | 2.20                     | 0.73              |
| 13:AM:19:LEU:HB3    | 13:AM:25:ILE:HG21  | 1.69                     | 0.73              |
| 10:AJ:50:ILE:HD11   | 14:AN:41:ARG:NH1   | 2.04                     | 0.73              |
| 22:AW:25:U:H2'      | 22:AW:26:C:C6      | 2.23                     | 0.73              |
| 32:B7:8:ASN:HD22    | 32:B7:9:ARG:N      | 1.86                     | 0.73              |
| 40:BF:65:TRP:HZ3    | 40:BF:75:HIS:HD2   | 1.34                     | 0.73              |
| 44:BK:57:ILE:HA     | 44:BK:66:THR:O     | 1.89                     | 0.73              |
| 58:BZ:119:GLU:O     | 58:BZ:121:HIS:N    | 2.20                     | 0.73              |
| 10:CJ:54:PHE:CG     | 10:CJ:55:LYS:HE3   | 2.23                     | 0.73              |
| 10:CJ:61:GLU:HG3    | 14:CN:58:LYS:NZ    | 2.03                     | 0.73              |
| 14:CN:23:ARG:HD2    | 14:CN:28:GLY:O     | 1.87                     | 0.73              |
| 31:D6:5:VAL:HG12    | 31:D6:6:ARG:O      | 1.88                     | 0.73              |
| 35:DA:1409:C:H2'    | 35:DA:1410:G:C8    | 2.23                     | 0.73              |
| 42:DH:18:GLU:HB2    | 42:DH:25:LYS:HB2   | 1.69                     | 0.73              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:DO:105:GLU:O    | 47:DO:109:LYS:HG2  | 1.87                     | 0.73              |
| 49:DQ:12:GLN:HE21  | 49:DQ:73:PRO:HD2   | 1.53                     | 0.73              |
| 52:DT:16:ARG:HD2   | 52:DT:18:ASP:OD1   | 1.88                     | 0.73              |
| 57:DY:8:LYS:HD2    | 57:DY:8:LYS:N      | 2.03                     | 0.73              |
| 49:DQ:108:GLY:HA3  | 58:DZ:116:VAL:HG11 | 1.69                     | 0.73              |
| 24:AY:121:VAL:HG23 | 24:AY:122:TRP:H    | 1.54                     | 0.73              |
| 28:B3:56:VAL:HG12  | 28:B3:57:GLU:H     | 1.51                     | 0.73              |
| 35:BA:1171:G:H2'   | 35:BA:1173:G:H4'   | 1.70                     | 0.73              |
| 25:B0:60:PHE:HE2   | 35:BA:2365:G:H4'   | 1.52                     | 0.73              |
| 36:BB:60:C:H2'     | 36:BB:61:G:H8      | 1.52                     | 0.73              |
| 40:BF:139:PHE:HB2  | 40:BF:166:ALA:HB1  | 1.69                     | 0.73              |
| 42:BH:96:ALA:HB1   | 42:BH:103:LEU:HD11 | 1.70                     | 0.73              |
| 44:BK:57:ILE:HD12  | 44:BK:57:ILE:H     | 1.53                     | 0.73              |
| 47:BO:105:GLU:O    | 47:BO:109:LYS:HG2  | 1.88                     | 0.73              |
| 52:BT:16:ARG:HD2   | 52:BT:18:ASP:OD1   | 1.88                     | 0.73              |
| 58:BZ:115:GLY:H    | 58:BZ:177:PRO:CG   | 2.01                     | 0.73              |
| 10:CJ:64:GLU:HG2   | 14:CN:59:ALA:HB2   | 1.71                     | 0.73              |
| 25:D0:25:ARG:HD2   | 25:D0:29:GLN:NE2   | 2.04                     | 0.73              |
| 26:D1:76:ARG:HH22  | 26:D1:95:LEU:CD1   | 2.00                     | 0.73              |
| 27:D2:38:GLN:HA    | 27:D2:41:ILE:HG23  | 1.69                     | 0.73              |
| 31:D6:27:LYS:HB3   | 31:D6:32:ASN:ND2   | 2.03                     | 0.73              |
| 31:D6:11:LEU:HD23  | 31:D6:51:GLU:HG3   | 1.70                     | 0.73              |
| 35:DA:2796:U:H3'   | 35:DA:2799:C:C5'   | 2.18                     | 0.73              |
| 35:DA:533:G:H5''   | 53:DU:24:TYR:CE2   | 2.23                     | 0.73              |
| 35:DA:991:C:H5'    | 35:DA:991:C:H6     | 1.53                     | 0.73              |
| 57:DY:96:ILE:HD12  | 57:DY:99:CYS:SG    | 2.29                     | 0.73              |
| 1:AA:1321:C:H5''   | 1:AA:1322:C:H5''   | 1.70                     | 0.73              |
| 12:AL:57:LYS:HG2   | 12:AL:67:THR:HG22  | 1.71                     | 0.73              |
| 18:AR:74:ARG:HB3   | 18:AR:81:PHE:CE2   | 2.23                     | 0.73              |
| 24:AY:157:LEU:H    | 24:AY:157:LEU:CD2  | 1.93                     | 0.73              |
| 24:AY:530:VAL:HG13 | 24:AY:531:GLY:H    | 1.53                     | 0.73              |
| 24:AY:514:VAL:HG21 | 24:AY:593:ALA:CB   | 2.18                     | 0.73              |
| 26:B1:81:LYS:C     | 26:B1:82:LEU:HD12  | 2.07                     | 0.73              |
| 35:BA:2122:U:H2'   | 35:BA:2123:G:C8    | 2.23                     | 0.73              |
| 35:BA:545:C:C3'    | 35:BA:547:A:H5''   | 2.19                     | 0.73              |
| 35:BA:83:G:HO2'    | 35:BA:84:A:H8      | 1.34                     | 0.73              |
| 39:BE:81:ILE:O     | 39:BE:81:ILE:HG22  | 1.88                     | 0.73              |
| 55:BW:68:ARG:O     | 55:BW:109:GLU:HA   | 1.89                     | 0.73              |
| 1:CA:1170:A:H2'    | 1:CA:1171:G:O4'    | 1.89                     | 0.73              |
| 3:CC:3:ASN:O       | 3:CC:4:LYS:HB2     | 1.89                     | 0.73              |
| 5:CE:51:VAL:HB     | 5:CE:52:PRO:HD3    | 1.70                     | 0.73              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 18:CR:74:ARG:HB3   | 18:CR:81:PHE:CE2    | 2.24                     | 0.73              |
| 25:D0:14:ARG:HB2   | 25:D0:14:ARG:HH11   | 1.54                     | 0.73              |
| 33:D8:56:GLU:O     | 33:D8:59:LYS:HE3    | 1.88                     | 0.73              |
| 35:DA:2461:C:O2    | 35:DA:2461:C:H2'    | 1.88                     | 0.73              |
| 36:DB:13:A:O2'     | 36:DB:14:U:H3'      | 1.88                     | 0.73              |
| 43:DJ:27:UNK:HA    | 43:DJ:112:UNK:O     | 1.87                     | 0.73              |
| 44:DK:57:ILE:HA    | 44:DK:66:THR:O      | 1.88                     | 0.73              |
| 58:DZ:128:VAL:HG21 | 58:DZ:132:ASN:HB2   | 1.69                     | 0.73              |
| 1:AA:1116:C:C2'    | 1:AA:1117:G:H5''    | 2.19                     | 0.73              |
| 1:AA:1239:A:H2'    | 1:AA:1298:C:N4      | 2.03                     | 0.73              |
| 1:AA:630:G:H2'     | 1:AA:631:G:C5'      | 2.19                     | 0.73              |
| 10:AJ:48:THR:HA    | 10:AJ:62:HIS:CB     | 2.17                     | 0.73              |
| 12:AL:47:LYS:HB3   | 12:AL:48:PRO:CD     | 2.19                     | 0.73              |
| 33:B8:4:MET:O      | 33:B8:62:LEU:HD12   | 1.89                     | 0.73              |
| 34:B9:32:HIS:O     | 34:B9:34:GLN:HG3    | 1.89                     | 0.73              |
| 35:BA:2132:U:C4    | 37:BC:6:LYS:HD2     | 2.24                     | 0.73              |
| 35:BA:272(H):C:H2' | 35:BA:272(I):U:H5'' | 1.70                     | 0.73              |
| 35:BA:2178:C:H4'   | 37:BC:47:LYS:HD3    | 1.70                     | 0.73              |
| 54:BV:77:ALA:O     | 54:BV:79:VAL:HG23   | 1.89                     | 0.73              |
| 58:BZ:23:LYS:HD3   | 58:BZ:38:TYR:CE1    | 2.23                     | 0.73              |
| 1:CA:598:U:H2'     | 1:CA:599:C:C6       | 2.24                     | 0.73              |
| 35:DA:272(H):C:H2' | 35:DA:272(I):U:H5'' | 1.71                     | 0.73              |
| 35:DA:2807:G:H1    | 35:DA:2893:G:H1     | 1.34                     | 0.73              |
| 35:DA:654(G):C:H2' | 35:DA:654(H):G:H8   | 1.51                     | 0.73              |
| 37:DC:128:LEU:O    | 37:DC:128:LEU:HG    | 1.87                     | 0.73              |
| 5:AE:76:ILE:HG13   | 5:AE:142:LEU:HD13   | 1.70                     | 0.73              |
| 22:AW:52:C:H2'     | 22:AW:53:G:O4'      | 1.89                     | 0.73              |
| 24:AY:227:ILE:HD11 | 24:AY:241:GLU:O     | 1.88                     | 0.73              |
| 24:AY:628:ARG:HH12 | 24:AY:680:PRO:HG2   | 1.53                     | 0.73              |
| 35:BA:1409:C:H2'   | 35:BA:1410:G:H8     | 1.51                     | 0.73              |
| 35:BA:364:C:H2'    | 35:BA:365:C:H5''    | 1.68                     | 0.73              |
| 38:BD:34:VAL:HG23  | 38:BD:35:LYS:N      | 2.04                     | 0.73              |
| 39:BE:34:VAL:O     | 39:BE:35:GLN:HB2    | 1.88                     | 0.73              |
| 35:BA:1080:C:H4'   | 44:BK:125:ARG:HB3   | 1.70                     | 0.73              |
| 35:BA:631:A:OP1    | 48:BP:64:LYS:HE2    | 1.88                     | 0.73              |
| 54:BV:28:GLU:HB2   | 54:BV:31:ALA:CB     | 2.19                     | 0.73              |
| 49:BQ:62:GLY:HA2   | 58:BZ:116:VAL:HG21  | 1.70                     | 0.73              |
| 58:BZ:142:SER:H    | 58:BZ:144:LEU:HD23  | 1.54                     | 0.73              |
| 1:CA:1004:A:N6     | 1:CA:1034:G:H2'     | 2.03                     | 0.73              |
| 1:CA:953:G:H5'     | 1:CA:965:A:H61      | 1.53                     | 0.73              |
| 12:CL:80:HIS:O     | 12:CL:81:SER:HB2    | 1.87                     | 0.73              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:CS:22:LEU:O     | 19:CS:26:GLY:HA2   | 1.89                     | 0.73              |
| 24:CY:678:GLU:HG2  | 24:CY:679:VAL:N    | 2.03                     | 0.73              |
| 25:D0:27:GLU:HA    | 25:D0:67:VAL:O     | 1.88                     | 0.73              |
| 35:DA:1378:A:H4'   | 35:DA:1379:A:OP1   | 1.87                     | 0.73              |
| 35:DA:1850:G:H5'   | 35:DA:1851:U:OP2   | 1.89                     | 0.73              |
| 35:DA:848:G:N3     | 35:DA:933:A:H1'    | 2.04                     | 0.73              |
| 35:DA:2579:C:C4'   | 39:DE:134:ILE:HG12 | 2.17                     | 0.73              |
| 1:AA:1219:U:H2'    | 1:AA:1220:G:C8     | 2.23                     | 0.72              |
| 1:AA:598:U:H2'     | 1:AA:599:C:C6      | 2.24                     | 0.72              |
| 4:AD:64:LEU:HB2    | 4:AD:198:VAL:HG11  | 1.71                     | 0.72              |
| 13:AM:3:ARG:HG2    | 13:AM:9:ILE:HD11   | 1.70                     | 0.72              |
| 24:AY:227:ILE:HG23 | 24:AY:237:PRO:CG   | 2.19                     | 0.72              |
| 24:AY:25:LYS:HE3   | 62:AY:703:GDP:O2B  | 1.89                     | 0.72              |
| 32:B7:24:THR:HG23  | 32:B7:27:GLY:H     | 1.54                     | 0.72              |
| 42:BH:41:MET:HG3   | 42:BH:43:VAL:HG13  | 1.71                     | 0.72              |
| 35:BA:662:G:OP1    | 48:BP:18:ARG:HD2   | 1.89                     | 0.72              |
| 50:BR:9:LYS:O      | 50:BR:10:LEU:HD23  | 1.88                     | 0.72              |
| 1:CA:630:G:H2'     | 1:CA:631:G:C5'     | 2.18                     | 0.72              |
| 2:CB:95:GLN:C      | 2:CB:96:ARG:HD2    | 2.10                     | 0.72              |
| 9:CI:47:LEU:N      | 9:CI:47:LEU:HD12   | 2.04                     | 0.72              |
| 33:D8:48:PHE:O     | 33:D8:49:VAL:HG22  | 1.88                     | 0.72              |
| 36:DB:60:C:H2'     | 36:DB:61:G:H8      | 1.53                     | 0.72              |
| 38:DD:155:LEU:HD23 | 38:DD:177:LEU:HD22 | 1.70                     | 0.72              |
| 52:DT:5:ALA:O      | 52:DT:7:ILE:N      | 2.22                     | 0.72              |
| 55:DW:10:VAL:HG23  | 55:DW:101:SER:O    | 1.89                     | 0.72              |
| 1:AA:103:C:H3'     | 1:AA:104:G:H8      | 1.54                     | 0.72              |
| 1:AA:178:C:O2'     | 1:AA:179:A:H5'     | 1.88                     | 0.72              |
| 1:AA:986:A:H1'     | 19:AS:54:GLY:O     | 1.89                     | 0.72              |
| 24:AY:512:ILE:H    | 24:AY:512:ILE:HD13 | 1.53                     | 0.72              |
| 35:BA:1540:U:H3'   | 35:BA:1541:G:H3'   | 1.70                     | 0.72              |
| 35:BA:1850:G:H5'   | 35:BA:1851:U:OP2   | 1.88                     | 0.72              |
| 27:B2:2:LYS:HB2    | 35:BA:97:C:H5''    | 1.69                     | 0.72              |
| 1:CA:1404:C:H1'    | 1:CA:1499:A:C2     | 2.24                     | 0.72              |
| 1:CA:353:A:H5'     | 1:CA:353:A:H8      | 1.54                     | 0.72              |
| 1:CA:552:U:H4'     | 12:CL:86:ARG:HG2   | 1.69                     | 0.72              |
| 19:CS:6:LYS:HG2    | 19:CS:7:LYS:HE3    | 1.71                     | 0.72              |
| 25:D0:77:ARG:HH22  | 35:DA:857:C:H5'    | 1.53                     | 0.72              |
| 35:DA:139:G:H1     | 35:DA:142(A):C:H42 | 1.34                     | 0.72              |
| 35:DA:1682:G:H2'   | 35:DA:1683:C:C6    | 2.23                     | 0.72              |
| 35:DA:654(S):G:H3' | 35:DA:654(T):C:C5' | 2.18                     | 0.72              |
| 36:DB:3:C:N4       | 36:DB:118:G:H1     | 1.86                     | 0.72              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:DU:95:LEU:HD13  | 54:DV:4:ILE:HG23   | 1.71                     | 0.72              |
| 1:AA:1133:G:H22    | 1:AA:1143:G:H1'    | 1.53                     | 0.72              |
| 1:AA:1513:A:H2'    | 1:AA:1514:C:C6     | 2.24                     | 0.72              |
| 1:AA:269:C:H2'     | 1:AA:270:A:C8      | 2.25                     | 0.72              |
| 7:AG:80:VAL:HG23   | 7:AG:81:GLY:H      | 1.54                     | 0.72              |
| 16:AP:74:LEU:CD2   | 16:AP:79:VAL:HG21  | 2.19                     | 0.72              |
| 28:B3:8:LEU:HD22   | 28:B3:31:LEU:CD2   | 2.18                     | 0.72              |
| 34:B9:36:GLN:OE1   | 35:BA:1124:C:H1'   | 1.90                     | 0.72              |
| 35:BA:1001:A:H2'   | 35:BA:1002:G:O4'   | 1.90                     | 0.72              |
| 35:BA:1203:G:H3'   | 35:BA:1204:A:H5''  | 1.71                     | 0.72              |
| 35:BA:139:G:H1     | 35:BA:142(A):C:H42 | 1.37                     | 0.72              |
| 35:BA:2258:C:O2'   | 35:BA:2426:A:H4'   | 1.89                     | 0.72              |
| 35:BA:2672:G:H2'   | 35:BA:2673:G:H5''  | 1.71                     | 0.72              |
| 35:BA:654(V):A:H3' | 35:BA:655:A:H2'    | 1.69                     | 0.72              |
| 42:BH:41:MET:O     | 42:BH:42:ARG:HB3   | 1.89                     | 0.72              |
| 1:CA:1321:C:H5''   | 1:CA:1322:C:H5''   | 1.71                     | 0.72              |
| 10:CJ:20:ALA:C     | 10:CJ:22:LYS:H     | 1.92                     | 0.72              |
| 16:CP:22:THR:HA    | 16:CP:33:ILE:HG12  | 1.69                     | 0.72              |
| 25:D0:27:GLU:N     | 25:D0:27:GLU:CD    | 2.41                     | 0.72              |
| 35:DA:1171:G:H2'   | 35:DA:1173:G:H4'   | 1.70                     | 0.72              |
| 39:DE:36:ARG:HH21  | 39:DE:88:GLY:CA    | 2.01                     | 0.72              |
| 42:DH:41:MET:O     | 42:DH:42:ARG:HB3   | 1.89                     | 0.72              |
| 53:DU:25:TRP:O     | 53:DU:28:ARG:HB2   | 1.89                     | 0.72              |
| 28:B3:56:VAL:HG12  | 28:B3:57:GLU:N     | 2.04                     | 0.72              |
| 33:B8:13:ARG:HD3   | 48:BP:61:ARG:O     | 1.87                     | 0.72              |
| 35:BA:2732:G:H3'   | 35:BA:2733:A:H5'   | 1.72                     | 0.72              |
| 35:BA:279:C:C3'    | 35:BA:280:C:H5''   | 2.20                     | 0.72              |
| 35:BA:395:U:H2'    | 35:BA:396:G:N7     | 2.05                     | 0.72              |
| 39:BE:61:ARG:HG2   | 39:BE:62:PRO:HD3   | 1.70                     | 0.72              |
| 54:BV:39:LEU:CD1   | 54:BV:51:VAL:HA    | 2.20                     | 0.72              |
| 1:CA:50:A:N6       | 1:CA:361:G:H4'     | 2.04                     | 0.72              |
| 3:CC:6:HIS:HD2     | 3:CC:7:PRO:HD2     | 1.54                     | 0.72              |
| 13:CM:78:ILE:HA    | 13:CM:81:LEU:HD23  | 1.70                     | 0.72              |
| 33:D8:54:GLU:O     | 33:D8:58:ILE:HG12  | 1.88                     | 0.72              |
| 35:DA:2315:G:O2'   | 41:DG:128:ARG:HD2  | 1.89                     | 0.72              |
| 35:DA:637:A:H2'    | 48:DP:117:GLU:OE2  | 1.89                     | 0.72              |
| 58:DZ:128:VAL:HG22 | 58:DZ:129:SER:N    | 2.04                     | 0.72              |
| 1:AA:1072:G:H2'    | 1:AA:1073:U:C6     | 2.25                     | 0.72              |
| 1:AA:1442:G:C6     | 1:AA:1442(B):A:H2  | 2.06                     | 0.72              |
| 3:AC:181:ASN:ND2   | 3:AC:204:LEU:HB2   | 2.03                     | 0.72              |
| 22:AW:31:G:H2'     | 22:AW:32:G:C8      | 2.23                     | 0.72              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:AY:468:ARG:CB  | 24:AY:468:ARG:HH11 | 2.01                     | 0.72              |
| 35:BA:1265:A:H5'  | 35:BA:1267:U:H1'   | 1.70                     | 0.72              |
| 35:BA:1827:C:O2'  | 35:BA:1828:G:H5'   | 1.89                     | 0.72              |
| 35:BA:2425:A:H4'  | 35:BA:2426:A:H5''  | 1.71                     | 0.72              |
| 37:BC:43:GLU:HG3  | 37:BC:216:THR:HG23 | 1.71                     | 0.72              |
| 40:BF:53:THR:HG22 | 40:BF:56:GLU:CG    | 2.14                     | 0.72              |
| 35:BA:674:G:H1'   | 40:BF:74:ARG:HD3   | 1.71                     | 0.72              |
| 42:BH:17:VAL:O    | 42:BH:45:VAL:HG22  | 1.88                     | 0.72              |
| 46:BN:65:LYS:HA   | 46:BN:65:LYS:HZ3   | 1.54                     | 0.72              |
| 52:BT:80:SER:HB3  | 52:BT:81:PRO:CD    | 2.19                     | 0.72              |
| 1:CA:631:G:H2'    | 1:CA:632:A:C8      | 2.23                     | 0.72              |
| 10:CJ:3:LYS:HZ2   | 10:CJ:76:ASN:HA    | 1.53                     | 0.72              |
| 13:CM:6:GLY:C     | 13:CM:8:GLU:H      | 1.91                     | 0.72              |
| 15:CO:11:VAL:O    | 15:CO:14:GLU:HB3   | 1.90                     | 0.72              |
| 22:CV:39:C:H2'    | 22:CV:40:C:C6      | 2.23                     | 0.72              |
| 24:CY:191:ASP:HA  | 24:CY:267:LYS:HE3  | 1.72                     | 0.72              |
| 25:D0:20:ARG:HD2  | 25:D0:20:ARG:H     | 1.54                     | 0.72              |
| 35:DA:176:G:O2'   | 35:DA:177:G:H5'    | 1.89                     | 0.72              |
| 35:DA:586:A:H5'   | 40:DF:89:VAL:HG21  | 1.69                     | 0.72              |
| 54:DV:15:GLU:HB3  | 54:DV:16:PRO:CD    | 2.18                     | 0.72              |
| 35:DA:64:A:C4     | 56:DX:66:LEU:HD13  | 2.24                     | 0.72              |
| 58:DZ:65:GLN:HB3  | 58:DZ:67:LEU:HD11  | 1.70                     | 0.72              |
| 4:AD:158:ILE:O    | 4:AD:162:LEU:HB2   | 1.89                     | 0.72              |
| 10:AJ:49:VAL:O    | 10:AJ:60:ARG:HB3   | 1.88                     | 0.72              |
| 19:AS:32:LYS:HA   | 19:AS:50:ALA:HB3   | 1.72                     | 0.72              |
| 19:AS:78:ARG:HB2  | 19:AS:81:ARG:HH11  | 1.52                     | 0.72              |
| 31:B6:40:CYS:HB2  | 31:B6:46:HIS:CE1   | 2.24                     | 0.72              |
| 33:B8:54:GLU:O    | 33:B8:58:ILE:HG12  | 1.90                     | 0.72              |
| 35:BA:1138:G:H2'  | 35:BA:1139:G:O4'   | 1.89                     | 0.72              |
| 35:BA:2198:A:H4'  | 35:BA:2199:A:OP1   | 1.88                     | 0.72              |
| 35:BA:2521:C:H42  | 35:BA:2544:G:H1    | 1.36                     | 0.72              |
| 35:BA:739:G:H4'   | 35:BA:740:U:OP1    | 1.89                     | 0.72              |
| 38:BD:183:ARG:HG2 | 38:BD:183:ARG:NH1  | 2.04                     | 0.72              |
| 35:BA:586:A:H5'   | 40:BF:89:VAL:HG21  | 1.71                     | 0.72              |
| 41:BG:135:LEU:CD1 | 41:BG:155:MET:HG2  | 2.18                     | 0.72              |
| 42:BH:20:ALA:HB1  | 42:BH:21:PRO:CD    | 2.18                     | 0.72              |
| 44:BK:75:SER:O    | 44:BK:79:ARG:HG3   | 1.90                     | 0.72              |
| 56:BX:41:ASN:O    | 56:BX:43:VAL:N     | 2.22                     | 0.72              |
| 24:CY:32:ILE:O    | 24:CY:36:THR:HG23  | 1.89                     | 0.72              |
| 35:DA:1430:C:H2'  | 35:DA:1431:U:C6    | 2.25                     | 0.72              |
| 35:DA:2198:A:H4'  | 35:DA:2199:A:OP1   | 1.89                     | 0.72              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:751:A:H5'    | 55:DW:90:ARG:HA    | 1.70                     | 0.72              |
| 39:DE:49:LEU:N     | 39:DE:49:LEU:HD22  | 2.03                     | 0.72              |
| 41:DG:116:ASP:O    | 41:DG:117:PHE:HB3  | 1.89                     | 0.72              |
| 55:DW:15:ARG:HA    | 55:DW:18:ARG:HD2   | 1.70                     | 0.72              |
| 6:AF:33:TYR:HB2    | 6:AF:75:LEU:HD13   | 1.70                     | 0.72              |
| 25:B0:14:ARG:HH11  | 25:B0:14:ARG:HB2   | 1.55                     | 0.72              |
| 26:B1:86:SER:CB    | 26:B1:89:GLU:HB2   | 2.18                     | 0.72              |
| 35:BA:1053:C:H2'   | 35:BA:1054:A:H5''  | 1.70                     | 0.72              |
| 46:BN:3:THR:HG22   | 46:BN:4:TYR:H      | 1.53                     | 0.72              |
| 48:BP:7:ARG:O      | 48:BP:10:PRO:HD2   | 1.89                     | 0.72              |
| 50:BR:7:GLY:O      | 50:BR:8:ARG:HB2    | 1.89                     | 0.72              |
| 58:BZ:103:ARG:HD2  | 58:BZ:136:PHE:CD1  | 2.24                     | 0.72              |
| 1:CA:1116:C:C2'    | 1:CA:1117:G:H5''   | 2.19                     | 0.72              |
| 1:CA:1296:C:H5'    | 1:CA:1297:C:OP2    | 1.88                     | 0.72              |
| 9:CI:40:LEU:HD11   | 9:CI:70:LYS:HG2    | 1.71                     | 0.72              |
| 12:CL:41:ARG:CG    | 12:CL:42:THR:H     | 2.02                     | 0.72              |
| 22:CV:2:G:H5''     | 25:D0:8:GLY:HA2    | 1.70                     | 0.72              |
| 35:DA:2306:C:H5''  | 35:DA:2307:G:O4'   | 1.89                     | 0.72              |
| 35:DA:365:C:H5'    | 35:DA:365:C:H6     | 1.54                     | 0.72              |
| 24:AY:92:ILE:HG12  | 24:AY:405:PRO:HG2  | 1.69                     | 0.72              |
| 35:BA:2150:U:H2'   | 35:BA:2151:G:C8    | 2.24                     | 0.72              |
| 35:BA:2461:C:O2    | 35:BA:2461:C:H2'   | 1.90                     | 0.72              |
| 41:BG:98:ARG:H     | 41:BG:98:ARG:HH11  | 1.37                     | 0.72              |
| 5:CE:7:GLU:HG2     | 5:CE:112:LEU:HD22  | 1.71                     | 0.72              |
| 24:CY:505:GLY:HA3  | 24:CY:576:ASP:CG   | 2.10                     | 0.72              |
| 35:DA:2732:G:H3'   | 35:DA:2733:A:H5'   | 1.71                     | 0.72              |
| 35:DA:320:A:H2'    | 40:DF:136:THR:OG1  | 1.90                     | 0.72              |
| 54:DV:15:GLU:CB    | 54:DV:16:PRO:HD2   | 2.20                     | 0.72              |
| 10:AJ:47:PHE:CZ    | 14:AN:37:PHE:HE2   | 2.07                     | 0.72              |
| 10:AJ:8:LEU:CD2    | 10:AJ:96:ILE:HG22  | 2.19                     | 0.72              |
| 24:AY:343:ASN:HD22 | 24:AY:344:THR:N    | 1.88                     | 0.72              |
| 35:BA:2455:G:H2'   | 35:BA:2456:C:C6    | 2.24                     | 0.72              |
| 45:BL:67:UNK:O     | 45:BL:69:UNK:N     | 2.23                     | 0.72              |
| 55:BW:4:LYS:HA     | 55:BW:106:ILE:HG22 | 1.72                     | 0.72              |
| 1:CA:1504:G:OP1    | 1:CA:1507:A:H4'    | 1.89                     | 0.72              |
| 13:CM:34:LEU:HD13  | 13:CM:41:PRO:HG3   | 1.72                     | 0.72              |
| 16:CP:32:TYR:HD2   | 16:CP:32:TYR:O     | 1.72                     | 0.72              |
| 29:D4:8:LYS:O      | 29:D4:9:LEU:HB2    | 1.87                     | 0.72              |
| 35:DA:154(A):C:H3' | 35:DA:155:U:C5'    | 2.20                     | 0.72              |
| 35:DA:2103:C:C3'   | 35:DA:2104:G:H5''  | 2.20                     | 0.72              |
| 44:DK:99:ILE:HD12  | 44:DK:103:GLN:HB3  | 1.71                     | 0.72              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 49:DQ:79:LEU:HD23 | 49:DQ:80:GLU:H    | 1.53                     | 0.72              |
| 54:DV:28:GLU:HB2  | 54:DV:31:ALA:CB   | 2.18                     | 0.72              |
| 58:DZ:9:TYR:HE2   | 58:DZ:61:LEU:HD22 | 1.54                     | 0.72              |
| 1:AA:1126:U:O4'   | 1:AA:1281:U:H1'   | 1.90                     | 0.72              |
| 1:AA:1352:C:H2'   | 1:AA:1353:G:C8    | 2.25                     | 0.72              |
| 1:AA:1423:G:C5'   | 47:BO:49:ARG:HH22 | 2.02                     | 0.72              |
| 1:AA:269:C:H2'    | 1:AA:270:A:H8     | 1.55                     | 0.72              |
| 10:AJ:64:GLU:HG2  | 14:AN:59:ALA:HB2  | 1.71                     | 0.72              |
| 12:AL:34:ARG:O    | 12:AL:61:THR:HG23 | 1.90                     | 0.72              |
| 18:AR:46:GLU:OE2  | 18:AR:46:GLU:HA   | 1.89                     | 0.72              |
| 35:BA:1787:A:H5'' | 35:BA:1788:C:OP2  | 1.90                     | 0.72              |
| 35:BA:297:C:H2'   | 35:BA:298:G:O4'   | 1.89                     | 0.72              |
| 35:BA:839:U:H2'   | 35:BA:840:C:C6    | 2.25                     | 0.72              |
| 38:BD:35:LYS:NZ   | 38:BD:36:PRO:HD3  | 2.01                     | 0.72              |
| 39:BE:11:MET:HB2  | 39:BE:23:VAL:O    | 1.89                     | 0.72              |
| 40:BF:178:PRO:HG2 | 40:BF:179:GLU:OE1 | 1.89                     | 0.72              |
| 46:BN:23:LEU:HB3  | 46:BN:60:ILE:HG21 | 1.70                     | 0.72              |
| 51:BS:96:GLY:O    | 51:BS:98:VAL:N    | 2.23                     | 0.72              |
| 55:BW:82:LEU:HD12 | 55:BW:82:LEU:N    | 2.05                     | 0.72              |
| 1:CA:294:U:H2'    | 1:CA:295:C:H6     | 1.55                     | 0.72              |
| 2:CB:168:THR:HG23 | 2:CB:192:SER:CB   | 2.17                     | 0.72              |
| 2:CB:22:LYS:H     | 2:CB:40:HIS:CE1   | 2.07                     | 0.72              |
| 7:CG:80:VAL:HG23  | 7:CG:81:GLY:H     | 1.55                     | 0.72              |
| 13:CM:3:ARG:HG2   | 13:CM:9:ILE:HD11  | 1.70                     | 0.72              |
| 19:CS:9:VAL:HG12  | 19:CS:9:VAL:O     | 1.90                     | 0.72              |
| 31:D6:47:THR:HG23 | 31:D6:48:VAL:H    | 1.55                     | 0.72              |
| 35:DA:184:C:H2'   | 35:DA:185:U:C6    | 2.25                     | 0.72              |
| 35:DA:2636:U:H4'  | 39:DE:80:GLU:OE1  | 1.90                     | 0.72              |
| 53:DU:59:ARG:HH11 | 53:DU:59:ARG:HG2  | 1.54                     | 0.72              |
| 4:AD:13:ARG:HA    | 4:AD:33:MET:HE1   | 1.73                     | 0.71              |
| 9:AI:17:VAL:HG11  | 9:AI:81:ILE:HD13  | 1.70                     | 0.71              |
| 9:AI:79:LEU:HD11  | 9:AI:83:ARG:HD2   | 1.72                     | 0.71              |
| 25:B0:27:GLU:HA   | 25:B0:67:VAL:O    | 1.89                     | 0.71              |
| 28:B3:40:THR:OG1  | 28:B3:43:ILE:HG12 | 1.89                     | 0.71              |
| 35:BA:745:G:H5'   | 35:BA:746:A:OP2   | 1.89                     | 0.71              |
| 1:CA:1100:C:H2'   | 1:CA:1101:A:H5''  | 1.72                     | 0.71              |
| 4:CD:64:LEU:HB2   | 4:CD:198:VAL:HG11 | 1.72                     | 0.71              |
| 10:CJ:4:ILE:N     | 10:CJ:4:ILE:HD12  | 2.04                     | 0.71              |
| 28:D3:56:VAL:HG12 | 28:D3:57:GLU:N    | 2.05                     | 0.71              |
| 35:DA:2020:A:O2'  | 35:DA:2021:C:H5'' | 1.90                     | 0.71              |
| 36:DB:7:G:C2'     | 36:DB:8:U:H5''    | 2.19                     | 0.71              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:DG:98:ARG:NH1   | 41:DG:98:ARG:HG2   | 2.04                     | 0.71              |
| 44:DK:99:ILE:HG23  | 44:DK:103:GLN:CB   | 2.20                     | 0.71              |
| 46:DN:3:THR:HG22   | 46:DN:4:TYR:H      | 1.55                     | 0.71              |
| 46:DN:96:GLU:OE2   | 46:DN:96:GLU:N     | 2.22                     | 0.71              |
| 56:DX:41:ASN:O     | 56:DX:43:VAL:N     | 2.22                     | 0.71              |
| 16:AP:32:TYR:O     | 16:AP:32:TYR:HD2   | 1.72                     | 0.71              |
| 24:AY:613:PRO:O    | 24:AY:615:GLU:N    | 2.23                     | 0.71              |
| 31:B6:11:LEU:HG    | 31:B6:26:ASN:HD21  | 1.55                     | 0.71              |
| 38:BD:243:GLY:O    | 38:BD:244:ARG:HB3  | 1.91                     | 0.71              |
| 48:BP:40:SER:C     | 48:BP:41:ARG:HD2   | 2.11                     | 0.71              |
| 48:BP:47:ASP:HB3   | 48:BP:48:PRO:CA    | 2.19                     | 0.71              |
| 18:CR:58:LEU:HB3   | 18:CR:62:GLU:HB3   | 1.71                     | 0.71              |
| 31:D6:40:CYS:HB2   | 31:D6:46:HIS:CE1   | 2.25                     | 0.71              |
| 35:DA:1203:G:H3'   | 35:DA:1204:A:H5''  | 1.72                     | 0.71              |
| 35:DA:1722:A:O2'   | 35:DA:1739:U:H5''  | 1.90                     | 0.71              |
| 35:DA:279:C:C3'    | 35:DA:280:C:H5''   | 2.20                     | 0.71              |
| 48:DP:59:LEU:HA    | 48:DP:61:ARG:CZ    | 2.20                     | 0.71              |
| 55:DW:4:LYS:HA     | 55:DW:106:ILE:HG22 | 1.72                     | 0.71              |
| 1:AA:108:G:H5'     | 1:AA:109:A:H5''    | 1.72                     | 0.71              |
| 1:AA:998:G:H2'     | 1:AA:999:C:C2      | 2.25                     | 0.71              |
| 2:AB:95:GLN:C      | 2:AB:96:ARG:HD2    | 2.11                     | 0.71              |
| 12:AL:7:ILE:O      | 12:AL:11:VAL:HG23  | 1.90                     | 0.71              |
| 35:BA:1819:A:H4'   | 35:BA:1820:U:C5'   | 2.20                     | 0.71              |
| 35:BA:2195:C:O2'   | 35:BA:2196:C:H5'   | 1.90                     | 0.71              |
| 35:BA:2439:A:N3    | 35:BA:2439:A:H2'   | 2.05                     | 0.71              |
| 37:BC:101:ILE:HG13 | 37:BC:128:LEU:HD11 | 1.71                     | 0.71              |
| 38:BD:158:ALA:O    | 38:BD:196:VAL:HG11 | 1.90                     | 0.71              |
| 1:CA:161:A:H2'     | 1:CA:162:A:C8      | 2.24                     | 0.71              |
| 10:CJ:44:VAL:HG22  | 10:CJ:66:ARG:HG2   | 1.71                     | 0.71              |
| 1:CA:973:G:H1'     | 10:CJ:55:LYS:CE    | 2.20                     | 0.71              |
| 10:CJ:8:LEU:CD2    | 10:CJ:96:ILE:HG22  | 2.19                     | 0.71              |
| 12:CL:47:LYS:HB3   | 12:CL:48:PRO:CD    | 2.19                     | 0.71              |
| 10:CJ:61:GLU:OE1   | 14:CN:49:HIS:HE1   | 1.74                     | 0.71              |
| 19:CS:51:VAL:O     | 19:CS:58:VAL:HG22  | 1.89                     | 0.71              |
| 24:CY:290:LYS:HB3  | 24:CY:298:VAL:HG23 | 1.72                     | 0.71              |
| 24:CY:605:ILE:HG23 | 24:CY:646:PHE:HB3  | 1.71                     | 0.71              |
| 31:D6:15:GLU:OE2   | 31:D6:44:ARG:NH1   | 2.23                     | 0.71              |
| 35:DA:1721:G:C6    | 35:DA:1739:U:H5'   | 2.25                     | 0.71              |
| 33:D8:2:PRO:HA     | 35:DA:591:C:O2     | 1.89                     | 0.71              |
| 35:DA:803:U:C2'    | 35:DA:804:A:H5'    | 2.20                     | 0.71              |
| 41:DG:173:LEU:O    | 41:DG:178:PHE:HB2  | 1.90                     | 0.71              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:DH:153:LYS:HG3  | 42:DH:154:PRO:HD2  | 1.70                     | 0.71              |
| 51:DS:12:PHE:O     | 51:DS:14:VAL:HG23  | 1.90                     | 0.71              |
| 52:DT:28:VAL:HG13  | 52:DT:46:GLU:HA    | 1.71                     | 0.71              |
| 49:DQ:62:GLY:HA2   | 58:DZ:116:VAL:HG21 | 1.72                     | 0.71              |
| 12:AL:34:ARG:HG3   | 12:AL:105:TYR:HE1  | 1.56                     | 0.71              |
| 35:BA:1061:U:H4'   | 35:BA:1070:A:H1'   | 1.72                     | 0.71              |
| 35:BA:2306:C:H5''  | 35:BA:2307:G:O4'   | 1.91                     | 0.71              |
| 35:BA:848:G:N3     | 35:BA:933:A:H1'    | 2.05                     | 0.71              |
| 35:BA:320:A:H2'    | 40:BF:136:THR:OG1  | 1.90                     | 0.71              |
| 40:BF:157:VAL:HG21 | 40:BF:194:MET:HG2  | 1.72                     | 0.71              |
| 42:BH:169:VAL:HG13 | 42:BH:170:ARG:N    | 2.04                     | 0.71              |
| 48:BP:27:HIS:CD2   | 48:BP:28:GLY:N     | 2.58                     | 0.71              |
| 48:BP:62:LEU:HD23  | 48:BP:62:LEU:N     | 2.06                     | 0.71              |
| 48:BP:62:LEU:N     | 48:BP:62:LEU:CD2   | 2.54                     | 0.71              |
| 54:BV:18:LEU:CD2   | 54:BV:19:LYS:H     | 2.02                     | 0.71              |
| 58:BZ:179:ASP:HB3  | 58:BZ:182:LYS:HD2  | 1.71                     | 0.71              |
| 1:CA:461:A:O2'     | 1:CA:470:C:H5'     | 1.91                     | 0.71              |
| 3:CC:84:ILE:O      | 3:CC:88:ARG:HG3    | 1.90                     | 0.71              |
| 4:CD:158:ILE:O     | 4:CD:162:LEU:HB2   | 1.89                     | 0.71              |
| 6:CF:33:TYR:HB2    | 6:CF:75:LEU:HD13   | 1.72                     | 0.71              |
| 22:CV:3:C:H42      | 22:CV:70:G:H1      | 1.35                     | 0.71              |
| 35:DA:582:G:H2'    | 35:DA:583:G:C8     | 2.26                     | 0.71              |
| 38:DD:35:LYS:C     | 38:DD:35:LYS:HD2   | 2.11                     | 0.71              |
| 46:DN:22:THR:O     | 46:DN:25:ARG:HB2   | 1.91                     | 0.71              |
| 35:DA:624:C:H41    | 48:DP:107:LYS:NZ   | 1.88                     | 0.71              |
| 57:DY:31:LEU:HB2   | 57:DY:32:PRO:HA    | 1.72                     | 0.71              |
| 1:AA:353:A:H5'     | 1:AA:353:A:H8      | 1.53                     | 0.71              |
| 1:AA:736:C:H2'     | 1:AA:737:A:C8      | 2.26                     | 0.71              |
| 3:AC:6:HIS:HD2     | 3:AC:7:PRO:HD2     | 1.55                     | 0.71              |
| 19:AS:15:LEU:HD21  | 19:AS:33:THR:OG1   | 1.90                     | 0.71              |
| 24:AY:180:VAL:HG23 | 24:AY:181:LEU:H    | 1.54                     | 0.71              |
| 29:B4:13:ARG:NH1   | 29:B4:13:ARG:HB3   | 2.06                     | 0.71              |
| 30:B5:55:ARG:HH22  | 50:BR:33:ARG:HG2   | 1.55                     | 0.71              |
| 31:B6:15:GLU:OE2   | 31:B6:44:ARG:NH2   | 2.23                     | 0.71              |
| 32:B7:23:ARG:C     | 32:B7:28:ARG:HH12  | 1.94                     | 0.71              |
| 35:BA:1682:G:H2'   | 35:BA:1683:C:C6    | 2.26                     | 0.71              |
| 35:BA:2466:C:O2'   | 35:BA:2467:C:H5'   | 1.91                     | 0.71              |
| 35:BA:500:G:N2     | 35:BA:502:A:H3'    | 2.06                     | 0.71              |
| 35:BA:756:C:O2'    | 35:BA:757:U:H5'    | 1.89                     | 0.71              |
| 35:BA:955:C:OP2    | 49:BQ:14:ARG:HD2   | 1.91                     | 0.71              |
| 35:BA:84:A:H5''    | 57:BY:9:LYS:HZ2    | 1.56                     | 0.71              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1298:C:H2'    | 1:CA:1298:C:O2     | 1.91                     | 0.71              |
| 1:CA:1382:C:H2'    | 1:CA:1383:C:H6     | 1.56                     | 0.71              |
| 2:CB:165:VAL:HG23  | 2:CB:166:ASP:N     | 2.04                     | 0.71              |
| 15:CO:5:LYS:O      | 15:CO:9:GLN:HG2    | 1.90                     | 0.71              |
| 18:CR:46:GLU:HA    | 18:CR:46:GLU:OE2   | 1.89                     | 0.71              |
| 24:CY:168:ILE:HD12 | 24:CY:176:GLY:HA3  | 1.72                     | 0.71              |
| 24:CY:608:VAL:O    | 24:CY:644:ARG:HA   | 1.91                     | 0.71              |
| 30:D5:4:HIS:CB     | 30:D5:5:PRO:HD3    | 2.19                     | 0.71              |
| 35:DA:2055:C:H4'   | 35:DA:2056:G:H5''  | 1.72                     | 0.71              |
| 35:DA:654(V):A:H3' | 35:DA:655:A:H2'    | 1.69                     | 0.71              |
| 38:DD:123:ALA:HB3  | 38:DD:131:LEU:HG   | 1.70                     | 0.71              |
| 39:DE:34:VAL:O     | 39:DE:35:GLN:HB2   | 1.89                     | 0.71              |
| 39:DE:61:ARG:HG2   | 39:DE:62:PRO:HD3   | 1.72                     | 0.71              |
| 44:DK:109:LYS:HA   | 44:DK:112:MET:CE   | 2.20                     | 0.71              |
| 47:DO:17:ARG:NE    | 47:DO:47:ILE:HD11  | 2.04                     | 0.71              |
| 1:AA:461:A:O2'     | 1:AA:470:C:H5'     | 1.90                     | 0.71              |
| 4:AD:200:GLU:H     | 4:AD:200:GLU:CD    | 1.94                     | 0.71              |
| 6:AF:37:VAL:HG12   | 6:AF:38:GLU:N      | 2.05                     | 0.71              |
| 10:AJ:92:THR:HG23  | 10:AJ:93:GLY:H     | 1.54                     | 0.71              |
| 16:AP:53:VAL:HG23  | 16:AP:54:GLU:H     | 1.54                     | 0.71              |
| 24:AY:459:LEU:H    | 24:AY:459:LEU:HD12 | 1.55                     | 0.71              |
| 29:B4:30:GLU:O     | 29:B4:31:ILE:HD12  | 1.90                     | 0.71              |
| 39:BE:38:THR:HG22  | 39:BE:40:GLU:N     | 2.03                     | 0.71              |
| 41:BG:56:ALA:HB1   | 41:BG:153:ARG:CZ   | 2.20                     | 0.71              |
| 47:BO:1:MET:HG3    | 47:BO:67:LYS:HG2   | 1.73                     | 0.71              |
| 51:BS:12:PHE:O     | 51:BS:14:VAL:HG23  | 1.90                     | 0.71              |
| 53:BU:20:LEU:CD2   | 53:BU:20:LEU:H     | 2.03                     | 0.71              |
| 12:CL:7:ILE:O      | 12:CL:11:VAL:HG23  | 1.90                     | 0.71              |
| 19:CS:9:VAL:O      | 19:CS:11:VAL:N     | 2.22                     | 0.71              |
| 26:D1:94:LEU:O     | 26:D1:96:LYS:N     | 2.23                     | 0.71              |
| 38:DD:27:THR:HG23  | 38:DD:83:GLU:HG2   | 1.72                     | 0.71              |
| 41:DG:62:LEU:CD1   | 41:DG:62:LEU:H     | 2.00                     | 0.71              |
| 35:DA:1190:G:H5'   | 48:DP:35:HIS:H     | 1.56                     | 0.71              |
| 49:DQ:35:VAL:HG23  | 49:DQ:101:ARG:O    | 1.91                     | 0.71              |
| 52:DT:28:VAL:HG22  | 52:DT:46:GLU:CA    | 2.21                     | 0.71              |
| 5:AE:98:THR:HB     | 5:AE:117:ASP:HB3   | 1.70                     | 0.71              |
| 10:AJ:61:GLU:OE1   | 14:AN:49:HIS:HE1   | 1.73                     | 0.71              |
| 16:AP:21:VAL:O     | 16:AP:33:ILE:HB    | 1.90                     | 0.71              |
| 19:AS:9:VAL:HG12   | 19:AS:9:VAL:O      | 1.88                     | 0.71              |
| 24:AY:180:VAL:CG2  | 24:AY:216:LEU:HD12 | 2.20                     | 0.71              |
| 24:AY:620:VAL:O    | 24:AY:624:LEU:HD13 | 1.89                     | 0.71              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:B6:47:THR:HG23  | 31:B6:48:VAL:H     | 1.56                     | 0.71              |
| 31:B6:5:VAL:CG2    | 35:BA:2283:C:H5'   | 2.18                     | 0.71              |
| 35:BA:2313:C:H5'   | 35:BA:2313:C:H6    | 1.54                     | 0.71              |
| 35:BA:614(A):U:H4' | 35:BA:614(B):G:C5' | 2.20                     | 0.71              |
| 38:BD:155:LEU:HD23 | 38:BD:177:LEU:HD22 | 1.72                     | 0.71              |
| 44:BK:99:ILE:HD12  | 44:BK:103:GLN:HB3  | 1.71                     | 0.71              |
| 57:BY:47:LYS:HG3   | 57:BY:60:PHE:HE2   | 1.54                     | 0.71              |
| 24:CY:84:THR:CA    | 61:CY:702:FUA:H322 | 2.20                     | 0.71              |
| 27:D2:22:GLU:O     | 27:D2:26:ARG:HG3   | 1.91                     | 0.71              |
| 35:DA:1709:U:H2'   | 35:DA:1710:C:C6    | 2.26                     | 0.71              |
| 35:DA:2171:A:H1'   | 35:DA:2172:U:C6    | 2.26                     | 0.71              |
| 35:DA:28:A:N6      | 35:DA:512:G:H1'    | 2.06                     | 0.71              |
| 37:DC:43:GLU:HG3   | 37:DC:216:THR:HG23 | 1.73                     | 0.71              |
| 47:DO:4:PRO:O      | 47:DO:5:GLN:HB2    | 1.91                     | 0.71              |
| 51:DS:98:VAL:C     | 51:DS:100:ALA:H    | 1.93                     | 0.71              |
| 57:DY:47:LYS:HG3   | 57:DY:60:PHE:HE2   | 1.54                     | 0.71              |
| 1:AA:1342:C:O2'    | 1:AA:1343:G:H5'    | 1.91                     | 0.71              |
| 13:AM:34:LEU:HD13  | 13:AM:41:PRO:HG3   | 1.72                     | 0.71              |
| 15:AO:11:VAL:O     | 15:AO:14:GLU:HB3   | 1.90                     | 0.71              |
| 35:BA:1582:C:H2'   | 35:BA:1583:A:H8    | 1.56                     | 0.71              |
| 35:BA:1709:U:H2'   | 35:BA:1710:C:C6    | 2.26                     | 0.71              |
| 35:BA:2103:C:C3'   | 35:BA:2104:G:H5''  | 2.20                     | 0.71              |
| 35:BA:2852:G:H2'   | 35:BA:2853:C:H6    | 1.56                     | 0.71              |
| 49:BQ:21:THR:O     | 49:BQ:22:LYS:HB3   | 1.90                     | 0.71              |
| 53:BU:25:TRP:O     | 53:BU:28:ARG:HB2   | 1.90                     | 0.71              |
| 44:BK:93:ARG:CG    | 58:BZ:112:ARG:HE   | 2.04                     | 0.71              |
| 1:CA:1133:G:H22    | 1:CA:1143:G:H1'    | 1.53                     | 0.71              |
| 1:CA:998:G:H2'     | 1:CA:999:C:C2      | 2.25                     | 0.71              |
| 8:CH:109:ILE:HG12  | 8:CH:110:ALA:N     | 2.05                     | 0.71              |
| 25:D0:30:VAL:HG12  | 25:D0:66:VAL:HG22  | 1.72                     | 0.71              |
| 41:DG:71:THR:HG22  | 41:DG:89:GLY:C     | 2.10                     | 0.71              |
| 44:DK:115:LEU:HD13 | 44:DK:126:MET:SD   | 2.30                     | 0.71              |
| 46:DN:65:LYS:HZ2   | 46:DN:65:LYS:HB3   | 1.55                     | 0.71              |
| 48:DP:40:SER:C     | 48:DP:41:ARG:HD2   | 2.10                     | 0.71              |
| 35:DA:955:C:OP2    | 49:DQ:14:ARG:HD2   | 1.89                     | 0.71              |
| 51:DS:89:ARG:HG3   | 51:DS:92:TYR:HA    | 1.73                     | 0.71              |
| 51:DS:95:HIS:CG    | 51:DS:96:GLY:H     | 2.07                     | 0.71              |
| 35:DA:84:A:H5''    | 57:DY:9:LYS:HZ2    | 1.56                     | 0.71              |
| 1:AA:1299:A:N3     | 1:AA:1299:A:H2'    | 2.05                     | 0.71              |
| 10:AJ:44:VAL:HG22  | 10:AJ:66:ARG:HG2   | 1.71                     | 0.71              |
| 35:BA:1721:G:C6    | 35:BA:1739:U:H5'   | 2.25                     | 0.71              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:2055:C:H4'   | 35:BA:2056:G:H5''  | 1.71                     | 0.71              |
| 35:BA:288:C:H2'    | 35:BA:289:A:C8     | 2.25                     | 0.71              |
| 27:B2:2:LYS:CB     | 35:BA:97:C:H5''    | 2.21                     | 0.71              |
| 36:BB:82:G:O2'     | 36:BB:83:G:H5'     | 1.91                     | 0.71              |
| 53:BU:90:VAL:O     | 53:BU:92:ARG:N     | 2.23                     | 0.71              |
| 56:BX:12:VAL:HG12  | 56:BX:27:THR:HG23  | 1.71                     | 0.71              |
| 1:CA:1486:G:H2'    | 1:CA:1487:G:O4'    | 1.90                     | 0.71              |
| 13:CM:3:ARG:HA     | 13:CM:9:ILE:HG13   | 1.73                     | 0.71              |
| 28:D3:17:LYS:HZ2   | 28:D3:20:LYS:HE3   | 1.55                     | 0.71              |
| 30:D5:2:ALA:N      | 35:DA:2014:A:HO2'  | 1.89                     | 0.71              |
| 31:D6:6:ARG:O      | 31:D6:7:ILE:HB     | 1.91                     | 0.71              |
| 33:D8:33:ASN:O     | 33:D8:34:TRP:HB3   | 1.91                     | 0.71              |
| 35:DA:2291:U:H2'   | 35:DA:2292:C:C6    | 2.25                     | 0.71              |
| 35:DA:500:G:N2     | 35:DA:502:A:H3'    | 2.06                     | 0.71              |
| 35:DA:803:U:O2'    | 35:DA:804:A:H5'    | 1.90                     | 0.71              |
| 41:DG:34:LEU:N     | 41:DG:34:LEU:HD12  | 2.04                     | 0.71              |
| 25:D0:7:LEU:CD1    | 49:DQ:85:LYS:HE2   | 2.21                     | 0.71              |
| 50:DR:63:ARG:NH2   | 50:DR:77:ARG:HG2   | 2.06                     | 0.71              |
| 53:DU:90:VAL:O     | 53:DU:92:ARG:N     | 2.24                     | 0.71              |
| 13:AM:90:LEU:O     | 13:AM:93:ARG:N     | 2.24                     | 0.71              |
| 19:AS:6:LYS:HG2    | 19:AS:7:LYS:HE3    | 1.71                     | 0.71              |
| 20:AT:12:ALA:O     | 20:AT:15:ARG:HB2   | 1.90                     | 0.71              |
| 33:B8:13:ARG:HH12  | 48:BP:59:LEU:HG    | 1.56                     | 0.71              |
| 35:BA:954:G:H4'    | 49:BQ:13:GLN:NE2   | 2.05                     | 0.71              |
| 38:BD:147:LEU:HD13 | 38:BD:155:LEU:HD11 | 1.71                     | 0.71              |
| 38:BD:77:ALA:HB2   | 38:BD:97:TYR:CD2   | 2.25                     | 0.71              |
| 46:BN:22:THR:HB    | 46:BN:25:ARG:HB2   | 1.73                     | 0.71              |
| 26:D1:61:ARG:HH11  | 26:D1:61:ARG:HB3   | 1.56                     | 0.71              |
| 27:D2:32:LEU:HD11  | 27:D2:54:LYS:HG2   | 1.73                     | 0.71              |
| 35:DA:2521:C:H42   | 35:DA:2544:G:H1    | 1.37                     | 0.71              |
| 39:DE:38:THR:HG22  | 39:DE:40:GLU:N     | 2.03                     | 0.71              |
| 41:DG:109:VAL:HG11 | 41:DG:142:PRO:HD3  | 1.72                     | 0.71              |
| 49:DQ:51:ARG:O     | 49:DQ:54:MET:HB3   | 1.89                     | 0.71              |
| 1:AA:973:G:H1'     | 10:AJ:55:LYS:CE    | 2.20                     | 0.70              |
| 10:AJ:61:GLU:HG3   | 14:AN:58:LYS:NZ    | 2.06                     | 0.70              |
| 15:AO:5:LYS:O      | 15:AO:9:GLN:HG2    | 1.91                     | 0.70              |
| 24:AY:154:GLN:HA   | 24:AY:158:GLY:HA2  | 1.72                     | 0.70              |
| 35:BA:1409:C:H2'   | 35:BA:1410:G:C8    | 2.26                     | 0.70              |
| 35:BA:2668:G:O2'   | 35:BA:2669:G:H5'   | 1.91                     | 0.70              |
| 35:BA:28:A:N6      | 35:BA:512:G:H1'    | 2.06                     | 0.70              |
| 35:BA:695:G:OP1    | 35:BA:1380:G:H4'   | 1.89                     | 0.70              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 35:BA:733:G:H8      | 35:BA:733:G:O5'    | 1.74                     | 0.70              |
| 40:BF:187:VAL:HG13  | 48:BP:5:ASP:O      | 1.91                     | 0.70              |
| 51:BS:98:VAL:HG12   | 51:BS:100:ALA:H    | 1.55                     | 0.70              |
| 55:BW:15:ARG:HA     | 55:BW:18:ARG:HD2   | 1.71                     | 0.70              |
| 3:CC:82:GLU:O       | 3:CC:86:VAL:HG13   | 1.90                     | 0.70              |
| 10:CJ:50:ILE:HD11   | 14:CN:41:ARG:NH1   | 2.05                     | 0.70              |
| 27:D2:61:LEU:HD12   | 35:DA:72:U:C6      | 2.26                     | 0.70              |
| 35:DA:1790:C:H5''   | 35:DA:1791:A:OP1   | 1.91                     | 0.70              |
| 35:DA:914:C:H2'     | 35:DA:915:C:H5'    | 1.71                     | 0.70              |
| 41:DG:60:LEU:HD22   | 41:DG:63:ILE:HD11  | 1.73                     | 0.70              |
| 44:DK:75:SER:O      | 44:DK:79:ARG:HG3   | 1.90                     | 0.70              |
| 48:DP:27:HIS:CD2    | 48:DP:28:GLY:N     | 2.59                     | 0.70              |
| 51:DS:89:ARG:O      | 51:DS:92:TYR:HB3   | 1.91                     | 0.70              |
| 22:AV:71:C:H2'      | 22:AV:71:C:O2      | 1.90                     | 0.70              |
| 24:AY:431:LEU:HD22  | 24:AY:466:LEU:HD13 | 1.72                     | 0.70              |
| 35:BA:158:U:H2'     | 35:BA:171:G:O4'    | 1.91                     | 0.70              |
| 35:BA:2133:G:C2'    | 35:BA:2157:G:H22   | 2.02                     | 0.70              |
| 35:BA:2291:U:H2'    | 35:BA:2292:C:C6    | 2.27                     | 0.70              |
| 35:BA:582:G:H2'     | 35:BA:583:G:C8     | 2.26                     | 0.70              |
| 35:BA:970:C:H2'     | 35:BA:971:C:C6     | 2.25                     | 0.70              |
| 36:BB:15:A:H3'      | 36:BB:16:G:H5'     | 1.73                     | 0.70              |
| 48:BP:79:ARG:O      | 48:BP:111:ARG:HB2  | 1.91                     | 0.70              |
| 58:BZ:29:TYR:HB3    | 58:BZ:34:ASN:HB2   | 1.73                     | 0.70              |
| 1:CA:1126:U:O4'     | 1:CA:1281:U:H1'    | 1.89                     | 0.70              |
| 1:CA:630:G:H2'      | 1:CA:631:G:H5'     | 1.73                     | 0.70              |
| 24:CY:568:TYR:CE2   | 24:CY:569:ASP:HB2  | 2.27                     | 0.70              |
| 35:DA:1138:G:H2'    | 35:DA:1139:G:O4'   | 1.90                     | 0.70              |
| 35:DA:1323:U:H3     | 35:DA:1331:A:H61   | 1.39                     | 0.70              |
| 35:DA:1367:A:H2'    | 35:DA:1368:G:H5'   | 1.72                     | 0.70              |
| 35:DA:1528(A):A:H62 | 35:DA:1541:G:N2    | 1.88                     | 0.70              |
| 35:DA:1819:A:H4'    | 35:DA:1820:U:C5'   | 2.21                     | 0.70              |
| 35:DA:1963:U:O2     | 35:DA:1963:U:H2'   | 1.89                     | 0.70              |
| 35:DA:2312:U:H2'    | 35:DA:2313:C:H5''  | 1.73                     | 0.70              |
| 35:DA:799:G:H3'     | 35:DA:800:A:H5''   | 1.73                     | 0.70              |
| 35:DA:85:G:OP1      | 57:DY:30:VAL:HB    | 1.92                     | 0.70              |
| 41:DG:76:SER:HB2    | 41:DG:83:ARG:CB    | 2.20                     | 0.70              |
| 35:DA:1080:C:H4'    | 44:DK:125:ARG:HB3  | 1.72                     | 0.70              |
| 48:DP:34:GLY:O      | 48:DP:35:HIS:HB2   | 1.90                     | 0.70              |
| 35:DA:958:U:OP2     | 49:DQ:14:ARG:NH1   | 2.25                     | 0.70              |
| 58:DZ:143:GLY:C     | 58:DZ:144:LEU:HD22 | 2.12                     | 0.70              |
| 10:AJ:20:ALA:C      | 10:AJ:22:LYS:H     | 1.91                     | 0.70              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 10:AJ:48:THR:HG23  | 10:AJ:62:HIS:ND1    | 2.06                     | 0.70              |
| 15:AO:39:LEU:HD13  | 15:AO:56:LEU:HB2    | 1.73                     | 0.70              |
| 26:B1:4:VAL:HG23   | 26:B1:10:LYS:O      | 1.92                     | 0.70              |
| 42:BH:175:LYS:O    | 42:BH:176:ALA:HB3   | 1.91                     | 0.70              |
| 1:CA:269:C:H2'     | 1:CA:270:A:H8       | 1.57                     | 0.70              |
| 1:CA:390:C:H2'     | 1:CA:391:G:C8       | 2.26                     | 0.70              |
| 10:CJ:82:ILE:O     | 10:CJ:86:MET:HB2    | 1.92                     | 0.70              |
| 24:CY:168:ILE:HD11 | 24:CY:178:ILE:CD1   | 2.22                     | 0.70              |
| 31:D6:16:CYS:SG    | 31:D6:48:VAL:HG21   | 2.31                     | 0.70              |
| 35:DA:1061:U:H4'   | 35:DA:1070:A:H1'    | 1.72                     | 0.70              |
| 35:DA:158:U:H2'    | 35:DA:171:G:O4'     | 1.91                     | 0.70              |
| 35:DA:1775:U:H2'   | 35:DA:1776:G:H5'    | 1.74                     | 0.70              |
| 46:DN:58:ASP:O     | 46:DN:60:ILE:N      | 2.24                     | 0.70              |
| 47:DO:1:MET:HG3    | 47:DO:67:LYS:HG2    | 1.74                     | 0.70              |
| 48:DP:16:ARG:NH1   | 48:DP:16:ARG:HB2    | 2.05                     | 0.70              |
| 51:DS:83:LYS:HG2   | 51:DS:105:ALA:HB3   | 1.73                     | 0.70              |
| 53:DU:107:ALA:HA   | 53:DU:110:VAL:CG2   | 2.22                     | 0.70              |
| 58:DZ:18:LEU:N     | 58:DZ:18:LEU:HD12   | 2.06                     | 0.70              |
| 58:DZ:18:LEU:CD1   | 58:DZ:18:LEU:H      | 2.03                     | 0.70              |
| 22:AW:14:A:C2'     | 22:AW:15:G:H5''     | 2.16                     | 0.70              |
| 24:AY:401:SER:O    | 24:AY:403:GLU:HG3   | 1.91                     | 0.70              |
| 27:B2:25:VAL:C     | 27:B2:27:GLU:H      | 1.93                     | 0.70              |
| 35:BA:2579:C:C4'   | 39:BE:134:ILE:HG12  | 2.19                     | 0.70              |
| 35:BA:1190:G:H5'   | 48:BP:35:HIS:H      | 1.55                     | 0.70              |
| 2:CB:167:PRO:HG2   | 2:CB:192:SER:OG     | 1.90                     | 0.70              |
| 10:CJ:7:LYS:O      | 10:CJ:96:ILE:HA     | 1.91                     | 0.70              |
| 13:CM:90:LEU:O     | 13:CM:93:ARG:N      | 2.24                     | 0.70              |
| 16:CP:49:LEU:HD22  | 16:CP:73:LEU:HD22   | 1.73                     | 0.70              |
| 24:CY:409:ILE:HD11 | 24:CY:656:ALA:HB3   | 1.72                     | 0.70              |
| 35:DA:1265:A:H5'   | 35:DA:1267:U:H1'    | 1.72                     | 0.70              |
| 35:DA:2308:G:O6    | 35:DA:2310:A:H2'    | 1.90                     | 0.70              |
| 35:DA:2258:C:O2'   | 35:DA:2426:A:H4'    | 1.90                     | 0.70              |
| 35:DA:2672:G:H2'   | 35:DA:2673:G:H5''   | 1.72                     | 0.70              |
| 35:DA:654(S):G:H3' | 35:DA:654(T):C:H5'' | 1.71                     | 0.70              |
| 35:DA:839:U:H2'    | 35:DA:840:C:C6      | 2.25                     | 0.70              |
| 35:DA:894:C:O2'    | 35:DA:895:U:H5'     | 1.91                     | 0.70              |
| 41:DG:131:TYR:HB3  | 41:DG:159:VAL:HG13  | 1.73                     | 0.70              |
| 48:DP:95:VAL:HG23  | 48:DP:125:VAL:HG23  | 1.73                     | 0.70              |
| 50:DR:10:LEU:HB3   | 50:DR:17:ARG:CD     | 2.21                     | 0.70              |
| 51:DS:97:ARG:NH2   | 51:DS:98:VAL:HA     | 2.06                     | 0.70              |
| 55:DW:68:ARG:O     | 55:DW:109:GLU:HA    | 1.91                     | 0.70              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:DZ:128:VAL:HG22 | 58:DZ:129:SER:H    | 1.54                     | 0.70              |
| 58:DZ:142:SER:H    | 58:DZ:144:LEU:HD23 | 1.54                     | 0.70              |
| 58:DZ:23:LYS:HD3   | 58:DZ:38:TYR:HE1   | 1.56                     | 0.70              |
| 1:AA:1170:A:H2'    | 1:AA:1171:G:O4'    | 1.91                     | 0.70              |
| 1:AA:161:A:H2'     | 1:AA:162:A:C8      | 2.26                     | 0.70              |
| 2:AB:22:LYS:H      | 2:AB:40:HIS:HE1    | 1.39                     | 0.70              |
| 8:AH:109:ILE:HG12  | 8:AH:110:ALA:N     | 2.06                     | 0.70              |
| 1:AA:1117:G:O2'    | 9:AI:104:ARG:HD3   | 1.90                     | 0.70              |
| 22:AW:69:C:H2'     | 22:AW:70:C:C6      | 2.27                     | 0.70              |
| 22:AW:7:G:H3'      | 22:AW:8:U:H5'      | 1.73                     | 0.70              |
| 31:B6:35:GLU:CB    | 31:B6:51:GLU:HB2   | 2.21                     | 0.70              |
| 41:BG:68:PRO:HA    | 41:BG:92:VAL:CG1   | 2.16                     | 0.70              |
| 42:BH:43:VAL:CG1   | 42:BH:52:VAL:HA    | 2.22                     | 0.70              |
| 44:BK:99:ILE:HG23  | 44:BK:103:GLN:CB   | 2.20                     | 0.70              |
| 44:BK:109:LYS:HA   | 44:BK:112:MET:CE   | 2.22                     | 0.70              |
| 44:BK:115:LEU:HD13 | 44:BK:126:MET:SD   | 2.31                     | 0.70              |
| 49:BQ:87:LYS:HG2   | 49:BQ:88:GLY:H     | 1.56                     | 0.70              |
| 35:DA:954:G:H4'    | 49:DQ:13:GLN:NE2   | 2.06                     | 0.70              |
| 38:DD:129:ASN:O    | 38:DD:193:VAL:HG12 | 1.91                     | 0.70              |
| 38:DD:77:ALA:HB2   | 38:DD:97:TYR:CD2   | 2.27                     | 0.70              |
| 1:AA:630:G:H2'     | 1:AA:631:G:H5'     | 1.74                     | 0.70              |
| 2:AB:153:ARG:C     | 2:AB:155:LEU:H     | 1.94                     | 0.70              |
| 10:AJ:8:LEU:HD23   | 10:AJ:96:ILE:HG22  | 1.72                     | 0.70              |
| 22:AV:20:U:C3'     | 22:AV:21:A:H5'     | 2.20                     | 0.70              |
| 22:AW:71:G:N3      | 22:AW:71:G:H2'     | 2.07                     | 0.70              |
| 25:B0:73:GLY:O     | 25:B0:75:LEU:N     | 2.24                     | 0.70              |
| 35:BA:894:C:O2'    | 35:BA:895:U:H5'    | 1.91                     | 0.70              |
| 37:BC:84:ILE:O     | 37:BC:95:VAL:HG11  | 1.91                     | 0.70              |
| 38:BD:65:ILE:HG22  | 38:BD:104:TYR:CB   | 2.18                     | 0.70              |
| 29:B4:9:LEU:CD2    | 41:BG:65:GLY:HA3   | 2.21                     | 0.70              |
| 47:BO:115:VAL:HG13 | 47:BO:121:VAL:HG21 | 1.72                     | 0.70              |
| 47:BO:4:PRO:O      | 47:BO:5:GLN:HB2    | 1.91                     | 0.70              |
| 48:BP:101:VAL:HG12 | 48:BP:106:LEU:HB3  | 1.74                     | 0.70              |
| 48:BP:16:ARG:NE    | 48:BP:18:ARG:HB2   | 2.07                     | 0.70              |
| 48:BP:85:LEU:CD1   | 48:BP:120:ALA:HB2  | 2.21                     | 0.70              |
| 51:BS:83:LYS:HG2   | 51:BS:105:ALA:HB3  | 1.73                     | 0.70              |
| 1:CA:60:A:H5''     | 1:CA:331:G:H22     | 1.56                     | 0.70              |
| 4:CD:4:TYR:O       | 4:CD:5:ILE:HB      | 1.90                     | 0.70              |
| 8:CH:17:THR:HB     | 8:CH:78:GLN:OE1    | 1.91                     | 0.70              |
| 10:CJ:8:LEU:HD23   | 10:CJ:96:ILE:HG22  | 1.74                     | 0.70              |
| 12:CL:34:ARG:HG3   | 12:CL:105:TYR:HE1  | 1.57                     | 0.70              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:CT:73:HIS:H     | 20:CT:76:ALA:HB3   | 1.55                     | 0.70              |
| 22:CW:74:A:C2'     | 22:CW:75:C:H5''    | 2.21                     | 0.70              |
| 25:D0:51:VAL:HG22  | 25:D0:81:VAL:HG23  | 1.72                     | 0.70              |
| 29:D4:13:ARG:HB3   | 29:D4:13:ARG:NH1   | 2.07                     | 0.70              |
| 29:D4:1:MET:HG2    | 41:DG:98:ARG:NE    | 2.07                     | 0.70              |
| 35:DA:120:U:O2     | 35:DA:120:U:H2'    | 1.89                     | 0.70              |
| 35:DA:88:G:OP1     | 35:DA:90:U:H5      | 1.74                     | 0.70              |
| 46:DN:22:THR:HB    | 46:DN:25:ARG:HB2   | 1.73                     | 0.70              |
| 47:DO:3:GLN:HB2    | 47:DO:4:PRO:HD2    | 1.73                     | 0.70              |
| 2:AB:107:THR:HA    | 2:AB:110:GLN:HE21  | 1.57                     | 0.70              |
| 2:AB:189:ASP:OD1   | 2:AB:205:ASP:HB3   | 1.91                     | 0.70              |
| 7:AG:120:ILE:HG22  | 7:AG:124:LEU:HD12  | 1.74                     | 0.70              |
| 14:AN:27:CYS:SG    | 14:AN:29:ARG:HB2   | 2.32                     | 0.70              |
| 24:AY:14:ASN:HB2   | 24:AY:102:ASP:OD1  | 1.91                     | 0.70              |
| 12:CL:57:LYS:HG2   | 12:CL:67:THR:HG22  | 1.74                     | 0.70              |
| 13:CM:15:VAL:O     | 13:CM:19:LEU:HD23  | 1.92                     | 0.70              |
| 1:CA:750:G:N3      | 15:CO:23:GLY:HA3   | 2.06                     | 0.70              |
| 24:CY:146:LEU:O    | 24:CY:149:VAL:HB   | 1.92                     | 0.70              |
| 35:DA:144:C:H2'    | 35:DA:145:G:H8     | 1.55                     | 0.70              |
| 35:DA:2415:G:O3'   | 48:DP:66:GLY:HA3   | 1.89                     | 0.70              |
| 35:DA:671:C:O2'    | 35:DA:672:C:H5'    | 1.91                     | 0.70              |
| 35:DA:742:G:O2'    | 35:DA:743:G:H5'    | 1.92                     | 0.70              |
| 27:D2:58:ALA:HB1   | 35:DA:76:C:H4'     | 1.74                     | 0.70              |
| 42:DH:169:VAL:HG13 | 42:DH:170:ARG:N    | 2.05                     | 0.70              |
| 52:DT:80:SER:HB3   | 52:DT:81:PRO:CD    | 2.20                     | 0.70              |
| 54:DV:39:LEU:CD1   | 54:DV:51:VAL:HA    | 2.22                     | 0.70              |
| 58:DZ:115:GLY:N    | 58:DZ:177:PRO:HG3  | 2.04                     | 0.70              |
| 1:AA:390:C:H2'     | 1:AA:391:G:C8      | 2.26                     | 0.70              |
| 10:AJ:7:LYS:O      | 10:AJ:96:ILE:HA    | 1.92                     | 0.70              |
| 11:AK:126:ARG:O    | 11:AK:128:ALA:N    | 2.25                     | 0.70              |
| 15:AO:82:ILE:HD13  | 15:AO:82:ILE:C     | 2.12                     | 0.70              |
| 61:AY:702:FUA:H122 | 61:AY:702:FUA:H231 | 1.73                     | 0.70              |
| 30:B5:2:ALA:N      | 35:BA:2014:A:HO2'  | 1.90                     | 0.70              |
| 35:BA:2171:A:H1'   | 35:BA:2172:U:C6    | 2.26                     | 0.70              |
| 35:BA:49:A:H5''    | 35:BA:51:G:O4'     | 1.92                     | 0.70              |
| 1:CA:986:A:H1'     | 19:CS:54:GLY:O     | 1.92                     | 0.70              |
| 12:CL:86:ARG:NH2   | 12:CL:99:HIS:CD2   | 2.59                     | 0.70              |
| 20:CT:49:ALA:HB1   | 20:CT:99:LEU:HG    | 1.72                     | 0.70              |
| 24:CY:492:ASP:OD1  | 24:CY:513:LYS:HA   | 1.92                     | 0.70              |
| 35:DA:1380:G:O2'   | 35:DA:1381:G:H5'   | 1.92                     | 0.70              |
| 51:DS:96:GLY:O     | 51:DS:98:VAL:HG23  | 1.91                     | 0.70              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:DU:55:ARG:HA    | 53:DU:58:ARG:CG    | 2.22                     | 0.70              |
| 1:AA:1358:U:OP1    | 14:AN:35:ARG:HG3   | 1.92                     | 0.70              |
| 24:AY:614:GLU:HB3  | 24:AY:617:MET:HE3  | 1.74                     | 0.70              |
| 25:B0:25:ARG:HD2   | 25:B0:29:GLN:NE2   | 2.06                     | 0.70              |
| 35:BA:1775:U:H2'   | 35:BA:1776:G:H5'   | 1.73                     | 0.70              |
| 39:BE:179:GLU:O    | 39:BE:180:ASN:HB2  | 1.92                     | 0.70              |
| 49:BQ:51:ARG:O     | 49:BQ:54:MET:HB3   | 1.91                     | 0.70              |
| 51:BS:74:ALA:HB1   | 51:BS:103:GLU:HB2  | 1.74                     | 0.70              |
| 51:BS:89:ARG:HG3   | 51:BS:92:TYR:HA    | 1.74                     | 0.70              |
| 52:BT:38:ASN:ND2   | 52:BT:38:ASN:C     | 2.40                     | 0.70              |
| 55:BW:33:ARG:O     | 55:BW:37:ARG:HB2   | 1.92                     | 0.70              |
| 1:CA:108:G:H5'     | 1:CA:109:A:H5''    | 1.74                     | 0.70              |
| 1:CA:1490:C:H2'    | 1:CA:1491:G:H5'    | 1.73                     | 0.70              |
| 1:CA:975:A:H5'     | 1:CA:975:A:C8      | 2.27                     | 0.70              |
| 9:CI:79:LEU:HD11   | 9:CI:83:ARG:HD2    | 1.72                     | 0.70              |
| 24:CY:339:SER:O    | 24:CY:351:ARG:HD2  | 1.91                     | 0.70              |
| 24:CY:487:ILE:HG22 | 24:CY:594:VAL:HG13 | 1.73                     | 0.70              |
| 26:D1:44:PRO:HG2   | 26:D1:46:LEU:CD2   | 2.19                     | 0.70              |
| 35:DA:695:G:OP1    | 35:DA:1380:G:H4'   | 1.92                     | 0.70              |
| 42:DH:41:MET:HG3   | 42:DH:43:VAL:HG13  | 1.72                     | 0.70              |
| 4:AD:189:PRO:HB2   | 4:AD:194:LEU:HD21  | 1.73                     | 0.70              |
| 13:AM:3:ARG:HA     | 13:AM:9:ILE:HG13   | 1.73                     | 0.70              |
| 22:AW:30:G:H2'     | 22:AW:31:G:C8      | 2.27                     | 0.70              |
| 35:BA:144:C:H2'    | 35:BA:145:G:H8     | 1.56                     | 0.70              |
| 35:BA:2262:U:C2'   | 35:BA:2263:C:C5'   | 2.70                     | 0.70              |
| 42:BH:89:ILE:HG23  | 42:BH:129:THR:O    | 1.91                     | 0.70              |
| 51:BS:96:GLY:O     | 51:BS:98:VAL:HG23  | 1.92                     | 0.70              |
| 54:BV:24:LYS:HA    | 54:BV:92:THR:HG23  | 1.73                     | 0.70              |
| 58:BZ:171:ILE:HG13 | 58:BZ:172:ALA:N    | 2.05                     | 0.70              |
| 4:CD:200:GLU:H     | 4:CD:200:GLU:CD    | 1.93                     | 0.70              |
| 12:CL:45:PRO:HG3   | 12:CL:53:ARG:HD3   | 1.74                     | 0.70              |
| 24:CY:7:TYR:OH     | 24:CY:9:LEU:HD12   | 1.92                     | 0.70              |
| 31:D6:15:GLU:OE2   | 31:D6:44:ARG:NH2   | 2.24                     | 0.70              |
| 35:DA:1846:G:H5'   | 35:DA:1846:G:C8    | 2.23                     | 0.70              |
| 42:DH:89:ILE:HG23  | 42:DH:129:THR:O    | 1.92                     | 0.70              |
| 54:DV:28:GLU:OE1   | 54:DV:31:ALA:HB2   | 1.92                     | 0.70              |
| 1:AA:1100:C:H2'    | 1:AA:1101:A:H5''   | 1.72                     | 0.69              |
| 1:AA:1329:A:P      | 13:AM:28:ALA:HB3   | 2.32                     | 0.69              |
| 1:AA:1346:A:H61    | 1:AA:1374:A:H3'    | 1.57                     | 0.69              |
| 2:AB:75:LYS:HA     | 2:AB:78:GLN:HG3    | 1.75                     | 0.69              |
| 2:AB:88:ALA:HB2    | 2:AB:219:VAL:HG13  | 1.74                     | 0.69              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 15:AO:55:GLY:HA2   | 15:AO:58:MET:HE3  | 1.73                     | 0.69              |
| 24:AY:252:ASP:HB2  | 24:AY:254:LYS:HG2 | 1.73                     | 0.69              |
| 35:BA:1323:U:H3    | 35:BA:1331:A:H61  | 1.40                     | 0.69              |
| 35:BA:1722:A:O2'   | 35:BA:1739:U:H5'' | 1.91                     | 0.69              |
| 35:BA:1884:A:H2'   | 35:BA:1885:A:C5'  | 2.20                     | 0.69              |
| 35:BA:2312:U:H2'   | 35:BA:2313:C:H5'' | 1.72                     | 0.69              |
| 36:BB:106:G:H5''   | 58:BZ:31:ARG:HB3  | 1.71                     | 0.69              |
| 38:BD:172:TYR:HD1  | 38:BD:186:HIS:HA  | 1.55                     | 0.69              |
| 41:BG:68:PRO:HB3   | 41:BG:90:LEU:HD11 | 1.74                     | 0.69              |
| 47:BO:2:ILE:HD11   | 47:BO:82:ASN:HD22 | 1.57                     | 0.69              |
| 47:BO:76:ALA:HB3   | 52:BT:75:ILE:HB   | 1.73                     | 0.69              |
| 48:BP:34:GLY:O     | 48:BP:35:HIS:HB2  | 1.92                     | 0.69              |
| 53:BU:95:LEU:HD13  | 54:BV:4:ILE:HG23  | 1.73                     | 0.69              |
| 55:BW:29:LEU:CD1   | 55:BW:51:LEU:HD11 | 2.21                     | 0.69              |
| 58:BZ:84:GLU:O     | 58:BZ:85:HIS:HB2  | 1.91                     | 0.69              |
| 1:CA:1161:C:H2'    | 1:CA:1162:C:C6    | 2.26                     | 0.69              |
| 1:CA:1299:A:N3     | 1:CA:1299:A:H2'   | 2.06                     | 0.69              |
| 1:CA:269:C:H2'     | 1:CA:270:A:C8     | 2.27                     | 0.69              |
| 8:CH:41:ARG:HH22   | 8:CH:123:GLU:CD   | 1.95                     | 0.69              |
| 15:CO:82:ILE:C     | 15:CO:82:ILE:HD13 | 2.12                     | 0.69              |
| 29:D4:30:GLU:O     | 29:D4:31:ILE:HD12 | 1.92                     | 0.69              |
| 36:DB:15:A:H3'     | 36:DB:16:G:H5'    | 1.72                     | 0.69              |
| 48:DP:16:ARG:NE    | 48:DP:18:ARG:HB2  | 2.06                     | 0.69              |
| 52:DT:24:PRO:HD3   | 52:DT:52:ILE:HD11 | 1.74                     | 0.69              |
| 3:AC:84:ILE:O      | 3:AC:88:ARG:HG3   | 1.92                     | 0.69              |
| 13:AM:23:TYR:HB3   | 13:AM:67:GLU:HB3  | 1.74                     | 0.69              |
| 24:AY:613:PRO:C    | 24:AY:615:GLU:H   | 1.94                     | 0.69              |
| 33:B8:23:VAL:HG12  | 33:B8:46:ARG:HH11 | 1.57                     | 0.69              |
| 35:BA:154(A):C:H3' | 35:BA:155:U:C5'   | 2.20                     | 0.69              |
| 35:BA:1599:C:H2'   | 35:BA:1600:C:H6   | 1.58                     | 0.69              |
| 35:BA:1607:C:H4'   | 35:BA:1608:A:O5'  | 1.92                     | 0.69              |
| 35:BA:2074:U:H2'   | 35:BA:2075:U:C6   | 2.27                     | 0.69              |
| 46:BN:22:THR:O     | 46:BN:25:ARG:HB2  | 1.91                     | 0.69              |
| 53:BU:59:ARG:HH11  | 53:BU:59:ARG:HG2  | 1.57                     | 0.69              |
| 1:CA:1049:U:H1'    | 1:CA:1201:A:N7    | 2.07                     | 0.69              |
| 1:CA:1490:C:C2'    | 1:CA:1491:G:H5'   | 2.22                     | 0.69              |
| 1:CA:736:C:H2'     | 1:CA:737:A:C8     | 2.27                     | 0.69              |
| 24:CY:514:VAL:HG21 | 24:CY:593:ALA:HB1 | 1.73                     | 0.69              |
| 26:D1:30:VAL:HG23  | 26:D1:31:GLY:H    | 1.56                     | 0.69              |
| 35:DA:1948:G:H5'   | 35:DA:1948:G:C8   | 2.27                     | 0.69              |
| 25:D0:16:SER:HB2   | 35:DA:2262:U:H5   | 1.56                     | 0.69              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1328:C:H2'    | 1:AA:1329:A:H8     | 1.58                     | 0.69              |
| 1:AA:793:U:C3'     | 1:AA:794:A:H5''    | 2.20                     | 0.69              |
| 2:AB:83:MET:HG3    | 2:AB:234:PRO:HG3   | 1.73                     | 0.69              |
| 11:AK:84:VAL:HG11  | 11:AK:95:ILE:HD11  | 1.74                     | 0.69              |
| 22:AV:5:G:N2       | 22:AV:69:C:C2      | 2.59                     | 0.69              |
| 24:AY:177:ILE:C    | 24:AY:178:ILE:HD12 | 2.11                     | 0.69              |
| 25:B0:30:VAL:HG12  | 25:B0:66:VAL:HG22  | 1.74                     | 0.69              |
| 30:B5:3:LYS:HD2    | 30:B5:5:PRO:HD2    | 1.72                     | 0.69              |
| 35:BA:2023:G:H5'   | 35:BA:2617:C:H4'   | 1.74                     | 0.69              |
| 35:BA:799:G:H3'    | 35:BA:800:A:H5''   | 1.74                     | 0.69              |
| 40:BF:7:TYR:HB3    | 40:BF:16:GLY:C     | 2.12                     | 0.69              |
| 52:BT:28:VAL:HG22  | 52:BT:46:GLU:CA    | 2.23                     | 0.69              |
| 1:CA:66:G:H4'      | 1:CA:173:U:C5      | 2.27                     | 0.69              |
| 1:CA:35:G:H2'      | 1:CA:36:C:C6       | 2.27                     | 0.69              |
| 4:CD:98:GLU:CG     | 4:CD:189:PRO:HG3   | 2.21                     | 0.69              |
| 10:CJ:71:LEU:HD12  | 10:CJ:72:VAL:H     | 1.57                     | 0.69              |
| 11:CK:126:ARG:O    | 11:CK:128:ALA:N    | 2.26                     | 0.69              |
| 15:CO:80:ALA:HB1   | 15:CO:84:LYS:HE2   | 1.73                     | 0.69              |
| 26:D1:56:GLN:HE22  | 26:D1:87:PRO:HB3   | 1.57                     | 0.69              |
| 35:DA:1607:C:H4'   | 35:DA:1608:A:O5'   | 1.92                     | 0.69              |
| 35:DA:2133:G:C2'   | 35:DA:2157:G:H22   | 2.02                     | 0.69              |
| 35:DA:566:U:O2'    | 35:DA:567:A:H5'    | 1.91                     | 0.69              |
| 36:DB:77:U:OP1     | 58:DZ:19:ARG:NH2   | 2.25                     | 0.69              |
| 37:DC:74:ARG:H     | 37:DC:112:ASP:HB2  | 1.57                     | 0.69              |
| 38:DD:261:LYS:HZ2  | 38:DD:263:ARG:HH12 | 1.38                     | 0.69              |
| 39:DE:81:ILE:O     | 39:DE:81:ILE:HG22  | 1.90                     | 0.69              |
| 40:DF:7:TYR:HB3    | 40:DF:16:GLY:C     | 2.12                     | 0.69              |
| 41:DG:110:ALA:HB1  | 41:DG:140:ILE:HD13 | 1.75                     | 0.69              |
| 42:DH:171:LEU:HD23 | 42:DH:172:LYS:O    | 1.90                     | 0.69              |
| 51:DS:17:ARG:O     | 51:DS:20:ARG:HG2   | 1.90                     | 0.69              |
| 1:AA:1038:C:H2'    | 1:AA:1039:C:C5     | 2.27                     | 0.69              |
| 1:AA:1473:A:O2'    | 1:AA:1474:G:H5'    | 1.92                     | 0.69              |
| 12:AL:18:VAL:HG23  | 12:AL:19:ARG:N     | 2.05                     | 0.69              |
| 35:BA:528:A:H2     | 35:BA:2043:C:H4'   | 1.56                     | 0.69              |
| 35:BA:825:C:O2'    | 35:BA:826:U:H5'    | 1.92                     | 0.69              |
| 35:BA:962:G:O2'    | 35:BA:963:U:H5'    | 1.92                     | 0.69              |
| 37:BC:115:VAL:HG12 | 37:BC:145:THR:HG23 | 1.74                     | 0.69              |
| 38:BD:153:ALA:O    | 38:BD:154:LYS:HG3  | 1.93                     | 0.69              |
| 38:BD:35:LYS:HD2   | 38:BD:36:PRO:CA    | 2.22                     | 0.69              |
| 42:BH:137:ASP:HB2  | 42:BH:140:LYS:HD2  | 1.74                     | 0.69              |
| 25:B0:7:LEU:HD22   | 49:BQ:81:VAL:HG23  | 1.74                     | 0.69              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:BT:28:VAL:HG13  | 52:BT:46:GLU:HA    | 1.74                     | 0.69              |
| 1:CA:1030(A):G:H1' | 1:CA:1031:G:H1     | 1.57                     | 0.69              |
| 26:D1:58:ILE:HD11  | 26:D1:91:LYS:HB2   | 1.74                     | 0.69              |
| 28:D3:40:THR:OG1   | 28:D3:43:ILE:HG12  | 1.92                     | 0.69              |
| 35:DA:1053:C:C2'   | 35:DA:1054:A:H5''  | 2.22                     | 0.69              |
| 35:DA:1582:C:H2'   | 35:DA:1583:A:H8    | 1.56                     | 0.69              |
| 35:DA:1787:A:H5''  | 35:DA:1788:C:OP2   | 1.92                     | 0.69              |
| 35:DA:2761:G:C3'   | 35:DA:2762:G:H5''  | 2.22                     | 0.69              |
| 43:DJ:13:UNK:C     | 43:DJ:15:UNK:H     | 2.05                     | 0.69              |
| 47:DO:115:VAL:HG13 | 47:DO:121:VAL:HG21 | 1.72                     | 0.69              |
| 49:DQ:3:MET:HB2    | 49:DQ:4:PRO:HD2    | 1.75                     | 0.69              |
| 25:D0:7:LEU:HD22   | 49:DQ:81:VAL:HG23  | 1.75                     | 0.69              |
| 50:DR:2:ARG:CD     | 50:DR:5:LYS:HE2    | 2.23                     | 0.69              |
| 47:DO:76:ALA:HB3   | 52:DT:75:ILE:HB    | 1.73                     | 0.69              |
| 1:AA:35:G:H2'      | 1:AA:36:C:C6       | 2.28                     | 0.69              |
| 1:AA:750:G:N3      | 15:AO:23:GLY:HA3   | 2.06                     | 0.69              |
| 1:AA:731:G:OP1     | 1:AA:766:A:H1'     | 1.93                     | 0.69              |
| 3:AC:70:VAL:HG12   | 3:AC:72:LYS:N      | 2.02                     | 0.69              |
| 4:AD:9:CYS:HA      | 4:AD:12:CYS:HB2    | 1.75                     | 0.69              |
| 6:AF:71:ARG:HG3    | 6:AF:71:ARG:HH11   | 1.57                     | 0.69              |
| 19:AS:20:LEU:HA    | 19:AS:23:ASN:HB2   | 1.74                     | 0.69              |
| 35:BA:1430:C:H2'   | 35:BA:1431:U:C6    | 2.28                     | 0.69              |
| 35:BA:2262:U:C2'   | 35:BA:2263:C:H5'   | 2.22                     | 0.69              |
| 35:BA:2593:U:H2'   | 35:BA:2594:C:C6    | 2.27                     | 0.69              |
| 35:BA:88:G:OP1     | 35:BA:90:U:H5      | 1.74                     | 0.69              |
| 35:BA:965:C:H5'    | 35:BA:2273:A:C1'   | 2.21                     | 0.69              |
| 39:BE:78:LEU:O     | 39:BE:79:ARG:HD2   | 1.91                     | 0.69              |
| 41:BG:95:ARG:O     | 41:BG:96:ARG:O     | 2.10                     | 0.69              |
| 47:BO:69:ILE:HD12  | 47:BO:69:ILE:N     | 2.08                     | 0.69              |
| 48:BP:84:ASN:HA    | 48:BP:115:LEU:O    | 1.92                     | 0.69              |
| 49:BQ:12:GLN:HE21  | 49:BQ:73:PRO:HD2   | 1.56                     | 0.69              |
| 51:BS:97:ARG:NH2   | 51:BS:98:VAL:HA    | 2.08                     | 0.69              |
| 10:CJ:13:HIS:O     | 10:CJ:17:ASP:HB2   | 1.93                     | 0.69              |
| 24:CY:84:THR:N     | 24:CY:85:PRO:HD3   | 2.05                     | 0.69              |
| 32:D7:8:ASN:HD22   | 32:D7:9:ARG:N      | 1.89                     | 0.69              |
| 35:DA:1884:A:H2'   | 35:DA:1885:A:C5'   | 2.20                     | 0.69              |
| 41:DG:75:LYS:O     | 41:DG:76:SER:HB3   | 1.92                     | 0.69              |
| 42:DH:137:ASP:HB2  | 42:DH:140:LYS:HD2  | 1.75                     | 0.69              |
| 1:AA:50:A:N6       | 1:AA:361:G:H4'     | 2.08                     | 0.69              |
| 2:AB:223:ILE:HA    | 2:AB:226:ARG:NE    | 2.08                     | 0.69              |
| 8:AH:41:ARG:HH22   | 8:AH:123:GLU:CD    | 1.94                     | 0.69              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 35:BA:2236:C:H2'    | 35:BA:2237:G:O4'   | 1.93                     | 0.69              |
| 35:BA:2801(A):A:H4' | 35:BA:2802:G:C8    | 2.28                     | 0.69              |
| 35:BA:671:C:O2'     | 35:BA:672:C:H5'    | 1.92                     | 0.69              |
| 37:BC:29:LEU:O      | 37:BC:32:GLU:HG2   | 1.93                     | 0.69              |
| 38:BD:27:THR:HG21   | 38:BD:83:GLU:HG2   | 1.72                     | 0.69              |
| 42:BH:43:VAL:HG11   | 42:BH:52:VAL:HA    | 1.74                     | 0.69              |
| 51:BS:70:GLY:C      | 51:BS:101:LEU:HD23 | 2.13                     | 0.69              |
| 53:BU:83:LEU:CD1    | 53:BU:83:LEU:H     | 2.06                     | 0.69              |
| 55:BW:10:VAL:HG23   | 55:BW:101:SER:O    | 1.93                     | 0.69              |
| 2:CB:107:THR:HA     | 2:CB:110:GLN:HE21  | 1.57                     | 0.69              |
| 2:CB:153:ARG:C      | 2:CB:155:LEU:H     | 1.95                     | 0.69              |
| 4:CD:28:SER:HB3     | 4:CD:29:PRO:HD2    | 1.73                     | 0.69              |
| 8:CH:42:GLU:HG3     | 8:CH:109:ILE:HD12  | 1.73                     | 0.69              |
| 24:CY:281:PRO:HB2   | 24:CY:286:ILE:HD11 | 1.74                     | 0.69              |
| 24:CY:90:PHE:HZ     | 61:CY:702:FUA:H121 | 1.57                     | 0.69              |
| 25:D0:40:GLN:HE22   | 25:D0:43:THR:HA    | 1.57                     | 0.69              |
| 30:D5:4:HIS:O       | 35:DA:2056:G:N2    | 2.25                     | 0.69              |
| 35:DA:395:U:H2'     | 35:DA:396:G:N7     | 2.06                     | 0.69              |
| 38:DD:172:TYR:CD1   | 38:DD:186:HIS:HA   | 2.27                     | 0.69              |
| 46:DN:26:LEU:C      | 46:DN:26:LEU:HD12  | 2.12                     | 0.69              |
| 53:DU:95:LEU:HD12   | 54:DV:11:GLN:HG3   | 1.75                     | 0.69              |
| 1:AA:1490:C:H6      | 1:AA:1490:C:C5'    | 2.06                     | 0.69              |
| 4:AD:28:SER:HB3     | 4:AD:29:PRO:HD2    | 1.74                     | 0.69              |
| 18:AR:58:LEU:HB3    | 18:AR:62:GLU:HB3   | 1.73                     | 0.69              |
| 24:AY:343:ASN:C     | 24:AY:343:ASN:HD22 | 1.96                     | 0.69              |
| 24:AY:71:THR:HG22   | 24:AY:80:ASN:OD1   | 1.93                     | 0.69              |
| 25:B0:19:LYS:HD3    | 25:B0:41:ARG:HH22  | 1.56                     | 0.69              |
| 31:B6:6:ARG:O       | 31:B6:7:ILE:HB     | 1.92                     | 0.69              |
| 33:B8:52:LYS:N      | 33:B8:53:PRO:CD    | 2.56                     | 0.69              |
| 35:BA:176:G:O2'     | 35:BA:177:G:H5'    | 1.93                     | 0.69              |
| 35:BA:582:G:H2'     | 35:BA:583:G:H8     | 1.58                     | 0.69              |
| 41:BG:131:TYR:HE2   | 41:BG:133:LEU:HB3  | 1.57                     | 0.69              |
| 44:BK:109:LYS:HA    | 44:BK:112:MET:HE2  | 1.74                     | 0.69              |
| 50:BR:10:LEU:HB3    | 50:BR:17:ARG:CD    | 2.22                     | 0.69              |
| 58:BZ:30:ASN:ND2    | 58:BZ:31:ARG:HG3   | 2.08                     | 0.69              |
| 1:CA:491:G:H2'      | 1:CA:492:G:H8      | 1.58                     | 0.69              |
| 2:CB:75:LYS:HA      | 2:CB:78:GLN:HG3    | 1.73                     | 0.69              |
| 3:CC:70:VAL:HG12    | 3:CC:72:LYS:N      | 2.00                     | 0.69              |
| 7:CG:120:ILE:HG22   | 7:CG:124:LEU:HD12  | 1.72                     | 0.69              |
| 10:CJ:49:VAL:CG2    | 14:CN:41:ARG:HB2   | 2.23                     | 0.69              |
| 19:CS:15:LEU:HD21   | 19:CS:33:THR:OG1   | 1.92                     | 0.69              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:CY:616:TYR:HE2  | 24:CY:664:GLN:HE21 | 1.40                     | 0.69              |
| 35:DA:614(A):U:H4' | 35:DA:614(B):G:C5' | 2.21                     | 0.69              |
| 40:DF:20:LEU:HD23  | 40:DF:21:ALA:N     | 2.08                     | 0.69              |
| 41:DG:16:ARG:O     | 41:DG:20:ILE:HG13  | 1.93                     | 0.69              |
| 48:DP:62:LEU:H     | 48:DP:62:LEU:CD2   | 2.06                     | 0.69              |
| 52:DT:129:ARG:O    | 52:DT:131:ALA:N    | 2.21                     | 0.69              |
| 55:DW:33:ARG:O     | 55:DW:37:ARG:HB2   | 1.92                     | 0.69              |
| 3:AC:175:LEU:HD21  | 3:AC:201:TYR:CE2   | 2.27                     | 0.69              |
| 22:AW:10:G:H2'     | 22:AW:11:A:H8      | 1.57                     | 0.69              |
| 22:AW:2:G:H1       | 22:AW:72:C:H42     | 1.40                     | 0.69              |
| 24:AY:416:LYS:HD3  | 24:AY:417:THR:H    | 1.56                     | 0.69              |
| 24:AY:555:LEU:HD11 | 24:AY:599:PRO:HB2  | 1.75                     | 0.69              |
| 31:B6:45:LYS:HD3   | 35:BA:2371:G:O3'   | 1.93                     | 0.69              |
| 35:BA:365:C:H5'    | 35:BA:365:C:H6     | 1.58                     | 0.69              |
| 35:BA:528:A:C2     | 35:BA:2043:C:H4'   | 2.27                     | 0.69              |
| 40:BF:154:VAL:HG11 | 40:BF:193:VAL:HG23 | 1.75                     | 0.69              |
| 35:BA:2415:G:O3'   | 48:BP:66:GLY:HA3   | 1.91                     | 0.69              |
| 35:BA:910:A:C5     | 49:BQ:13:GLN:HG3   | 2.27                     | 0.69              |
| 1:CA:1310:G:O2'    | 1:CA:1311:G:H5'    | 1.93                     | 0.69              |
| 3:CC:206:GLU:HG2   | 3:CC:207:VAL:H     | 1.56                     | 0.69              |
| 11:CK:48:ILE:HG22  | 11:CK:49:GLY:H     | 1.57                     | 0.69              |
| 12:CL:23:LYS:O     | 12:CL:24:VAL:HG23  | 1.92                     | 0.69              |
| 14:CN:27:CYS:SG    | 14:CN:29:ARG:HB2   | 2.31                     | 0.69              |
| 20:CT:12:ALA:O     | 20:CT:15:ARG:HB2   | 1.93                     | 0.69              |
| 24:CY:210:ARG:HH11 | 24:CY:210:ARG:HG2  | 1.56                     | 0.69              |
| 35:DA:1099:G:H2'   | 35:DA:1100:C:O4'   | 1.93                     | 0.69              |
| 35:DA:2023:G:H5'   | 35:DA:2617:C:H4'   | 1.74                     | 0.69              |
| 35:DA:2236:C:H2'   | 35:DA:2237:G:O4'   | 1.93                     | 0.69              |
| 35:DA:2753:A:O2'   | 35:DA:2754:U:H5'   | 1.92                     | 0.69              |
| 35:DA:582:G:H2'    | 35:DA:583:G:H8     | 1.56                     | 0.69              |
| 37:DC:78:ILE:O     | 37:DC:120:VAL:HG21 | 1.93                     | 0.69              |
| 37:DC:84:ILE:O     | 37:DC:95:VAL:HG11  | 1.93                     | 0.69              |
| 42:DH:43:VAL:CG1   | 42:DH:52:VAL:HA    | 2.22                     | 0.69              |
| 52:DT:107:ASP:CG   | 52:DT:108:ARG:H    | 1.95                     | 0.69              |
| 55:DW:82:LEU:N     | 55:DW:82:LEU:HD12  | 2.07                     | 0.69              |
| 1:AA:1030(A):G:H1' | 1:AA:1031:G:H1     | 1.57                     | 0.69              |
| 1:AA:1226:C:H5'    | 13:AM:96:LEU:HD13  | 1.74                     | 0.69              |
| 1:AA:625:G:H4'     | 16:AP:16:HIS:CD2   | 2.28                     | 0.69              |
| 19:AS:51:VAL:O     | 19:AS:58:VAL:HG22  | 1.93                     | 0.69              |
| 20:AT:49:ALA:HB1   | 20:AT:99:LEU:HG    | 1.73                     | 0.69              |
| 24:AY:261:GLY:HA3  | 24:AY:267:LYS:O    | 1.93                     | 0.69              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:AY:272:LEU:O    | 24:AY:275:ALA:HB3  | 1.92                     | 0.69              |
| 24:AY:554:PRO:HG3  | 24:AY:594:VAL:HG12 | 1.74                     | 0.69              |
| 29:B4:12:ALA:CB    | 29:B4:29:PRO:HA    | 2.23                     | 0.69              |
| 30:B5:45:VAL:HG22  | 30:B5:51:TYR:CE1   | 2.28                     | 0.69              |
| 36:BB:20:C:O2'     | 36:BB:21:G:H5''    | 1.92                     | 0.69              |
| 39:BE:179:GLU:HB3  | 39:BE:181:LEU:HD23 | 1.73                     | 0.69              |
| 41:BG:32:PRO:HA    | 41:BG:162:THR:HB   | 1.75                     | 0.69              |
| 35:BA:2012:G:C4'   | 55:BW:96:ILE:HD11  | 2.15                     | 0.69              |
| 8:CH:10:LEU:HD22   | 8:CH:83:ILE:HD11   | 1.73                     | 0.69              |
| 18:CR:29:PHE:N     | 18:CR:29:PHE:CD2   | 2.56                     | 0.69              |
| 24:CY:157:LEU:CD2  | 24:CY:157:LEU:H    | 2.05                     | 0.69              |
| 24:CY:228:MET:O    | 24:CY:231:TYR:HB3  | 1.93                     | 0.69              |
| 27:D2:40:SER:C     | 27:D2:42:GLY:H     | 1.95                     | 0.69              |
| 30:D5:45:VAL:HG22  | 30:D5:51:TYR:CE1   | 2.28                     | 0.69              |
| 35:DA:2524:G:C8    | 35:DA:2524:G:H5'   | 2.25                     | 0.69              |
| 35:DA:272(I):U:O2  | 35:DA:272(I):U:H3' | 1.93                     | 0.69              |
| 37:DC:29:LEU:O     | 37:DC:32:GLU:HG2   | 1.93                     | 0.69              |
| 38:DD:106:ILE:HD11 | 38:DD:196:VAL:HG13 | 1.75                     | 0.69              |
| 38:DD:27:THR:HG21  | 38:DD:83:GLU:HG2   | 1.72                     | 0.69              |
| 41:DG:41:GLN:HG2   | 41:DG:155:MET:HB3  | 1.73                     | 0.69              |
| 46:DN:45:ASN:HD22  | 46:DN:45:ASN:N     | 1.86                     | 0.69              |
| 55:DW:78:GLU:OE2   | 55:DW:99:ARG:HD2   | 1.93                     | 0.69              |
| 58:DZ:10:ARG:NH2   | 58:DZ:26:GLY:N     | 2.40                     | 0.69              |
| 1:AA:1382:C:H2'    | 1:AA:1383:C:H6     | 1.56                     | 0.69              |
| 1:AA:627:G:O2'     | 1:AA:628:G:H5'     | 1.93                     | 0.69              |
| 24:AY:539:ILE:HA   | 24:AY:542:VAL:HG12 | 1.74                     | 0.69              |
| 35:BA:184:C:H2'    | 35:BA:185:U:C6     | 2.27                     | 0.69              |
| 35:BA:2105:C:H42   | 35:BA:2184:G:H1    | 1.40                     | 0.69              |
| 38:BD:123:ALA:HB3  | 38:BD:131:LEU:HG   | 1.75                     | 0.69              |
| 38:BD:27:THR:HG23  | 38:BD:83:GLU:HG2   | 1.74                     | 0.69              |
| 49:BQ:3:MET:HB2    | 49:BQ:4:PRO:HD2    | 1.75                     | 0.69              |
| 56:BX:12:VAL:HB    | 56:BX:17:ALA:CB    | 2.12                     | 0.69              |
| 57:BY:31:LEU:HB2   | 57:BY:32:PRO:HA    | 1.73                     | 0.69              |
| 1:CA:627:G:O2'     | 1:CA:628:G:H5'     | 1.91                     | 0.69              |
| 2:CB:222:ILE:HB    | 2:CB:226:ARG:HH21  | 1.57                     | 0.69              |
| 10:CJ:16:LEU:O     | 10:CJ:16:LEU:HD13  | 1.93                     | 0.69              |
| 11:CK:23:ALA:HB1   | 11:CK:88:GLY:HA3   | 1.73                     | 0.69              |
| 1:CA:1226:C:H5'    | 13:CM:96:LEU:HD13  | 1.74                     | 0.69              |
| 24:CY:103:GLY:O    | 24:CY:104:ALA:HB2  | 1.92                     | 0.69              |
| 25:D0:19:LYS:HD3   | 25:D0:41:ARG:HH22  | 1.58                     | 0.69              |
| 25:D0:73:GLY:O     | 25:D0:75:LEU:N     | 2.23                     | 0.69              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:D2:33:MET:O     | 27:D2:37:PHE:HB2  | 1.92                     | 0.69              |
| 35:DA:1010:A:H1'   | 35:DA:1153:C:H1'  | 1.75                     | 0.69              |
| 35:DA:1639:U:O2'   | 35:DA:1640:C:H5'' | 1.92                     | 0.69              |
| 35:DA:1779:U:C5    | 35:DA:1784:A:N7   | 2.58                     | 0.69              |
| 36:DB:20:C:O2'     | 36:DB:21:G:H5''   | 1.92                     | 0.69              |
| 38:DD:91:ARG:HG2   | 38:DD:91:ARG:NH1  | 2.04                     | 0.69              |
| 52:DT:129:ARG:O    | 52:DT:129:ARG:HG2 | 1.93                     | 0.69              |
| 12:AL:17:LYS:HD3   | 12:AL:18:VAL:HG22 | 1.74                     | 0.69              |
| 15:AO:56:LEU:O     | 15:AO:60:VAL:HG23 | 1.93                     | 0.69              |
| 19:AS:6:LYS:CE     | 19:AS:6:LYS:H     | 2.05                     | 0.69              |
| 33:B8:6:THR:CG2    | 33:B8:63:PRO:HD3  | 2.23                     | 0.69              |
| 35:BA:1504:C:H2'   | 35:BA:1505:C:H5'' | 1.74                     | 0.69              |
| 40:BF:43:LYS:HA    | 40:BF:98:SER:HB3  | 1.74                     | 0.69              |
| 41:BG:138:GLN:OE1  | 41:BG:153:ARG:HG2 | 1.92                     | 0.69              |
| 41:BG:67:LYS:HD3   | 41:BG:68:PRO:N    | 2.08                     | 0.69              |
| 50:BR:2:ARG:CD     | 50:BR:5:LYS:HE2   | 2.23                     | 0.69              |
| 1:CA:1325:C:H2'    | 1:CA:1326:C:H6    | 1.56                     | 0.69              |
| 3:CC:148:GLY:HA3   | 3:CC:172:ARG:O    | 1.92                     | 0.69              |
| 3:CC:150:LYS:HB2   | 3:CC:169:ALA:HB1  | 1.75                     | 0.69              |
| 4:CD:160:GLN:O     | 4:CD:163:GLU:HB3  | 1.91                     | 0.69              |
| 11:CK:108:ILE:HD12 | 11:CK:108:ILE:N   | 2.08                     | 0.69              |
| 19:CS:44:MET:N     | 19:CS:44:MET:SD   | 2.66                     | 0.69              |
| 26:D1:19:GLN:O     | 26:D1:35:THR:HG22 | 1.92                     | 0.69              |
| 26:D1:76:ARG:NH2   | 26:D1:95:LEU:HB2  | 2.08                     | 0.69              |
| 35:DA:2262:U:C2'   | 35:DA:2263:C:C5'  | 2.71                     | 0.69              |
| 35:DA:2807:G:C3'   | 35:DA:2808:U:H5'' | 2.22                     | 0.69              |
| 35:DA:419:C:H2'    | 35:DA:420:C:H6    | 1.56                     | 0.69              |
| 40:DF:187:VAL:HG13 | 48:DP:5:ASP:O     | 1.92                     | 0.69              |
| 40:DF:195:ASP:OD1  | 40:DF:196:LEU:N   | 2.22                     | 0.69              |
| 51:DS:74:ALA:HB1   | 51:DS:103:GLU:HB2 | 1.74                     | 0.69              |
| 1:AA:975:A:H5'     | 1:AA:975:A:C8     | 2.28                     | 0.68              |
| 13:AM:78:ILE:O     | 13:AM:82:MET:HG2  | 1.93                     | 0.68              |
| 1:AA:1358:U:P      | 14:AN:35:ARG:HG3  | 2.33                     | 0.68              |
| 20:AT:73:HIS:H     | 20:AT:76:ALA:HB3  | 1.56                     | 0.68              |
| 24:AY:12:LEU:O     | 24:AY:283:PRO:HD3 | 1.92                     | 0.68              |
| 31:B6:30:THR:O     | 31:B6:32:ASN:N    | 2.25                     | 0.68              |
| 33:B8:56:GLU:O     | 33:B8:59:LYS:HE3  | 1.92                     | 0.68              |
| 34:B9:1:MET:O      | 34:B9:34:GLN:HG2  | 1.93                     | 0.68              |
| 35:BA:2753:A:O2'   | 35:BA:2754:U:H5'  | 1.93                     | 0.68              |
| 40:BF:20:LEU:HD23  | 40:BF:21:ALA:N    | 2.08                     | 0.68              |
| 41:BG:111:LEU:HA   | 41:BG:114:ILE:CD1 | 2.22                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 48:BP:59:LEU:HA     | 48:BP:61:ARG:CZ    | 2.22                     | 0.68              |
| 52:BT:23:ARG:HB2    | 52:BT:24:PRO:HD2   | 1.75                     | 0.68              |
| 52:BT:45:PHE:CE2    | 52:BT:74:ARG:HB2   | 2.28                     | 0.68              |
| 58:BZ:120:ILE:O     | 58:BZ:121:HIS:HB2  | 1.93                     | 0.68              |
| 58:BZ:137:ILE:HG21  | 58:BZ:155:LEU:HD12 | 1.75                     | 0.68              |
| 1:CA:460:G:H5'      | 1:CA:461:A:OP2     | 1.93                     | 0.68              |
| 13:CM:23:TYR:HB3    | 13:CM:67:GLU:HB3   | 1.75                     | 0.68              |
| 13:CM:78:ILE:O      | 13:CM:82:MET:HG2   | 1.94                     | 0.68              |
| 24:CY:392:GLU:HG3   | 24:CY:393:ASP:OD1  | 1.93                     | 0.68              |
| 27:D2:55:ARG:O      | 27:D2:58:ALA:HB3   | 1.92                     | 0.68              |
| 35:DA:1345:C:O2'    | 35:DA:1346:G:H5'   | 1.94                     | 0.68              |
| 35:DA:2439:A:H2'    | 35:DA:2439:A:N3    | 2.07                     | 0.68              |
| 35:DA:2801(A):A:H4' | 35:DA:2802:G:C8    | 2.28                     | 0.68              |
| 40:DF:157:VAL:HG21  | 40:DF:194:MET:HG2  | 1.74                     | 0.68              |
| 49:DQ:97:VAL:HG11   | 49:DQ:103:MET:CE   | 2.23                     | 0.68              |
| 54:DV:19:LYS:HG2    | 54:DV:94:LEU:HB2   | 1.75                     | 0.68              |
| 54:DV:24:LYS:HA     | 54:DV:92:THR:HG23  | 1.73                     | 0.68              |
| 1:AA:235:C:H5'      | 17:AQ:70:ARG:HG2   | 1.73                     | 0.68              |
| 1:AA:697:U:C2'      | 1:AA:698:G:H5'     | 2.23                     | 0.68              |
| 4:AD:162:LEU:HD11   | 4:AD:181:MET:HG2   | 1.73                     | 0.68              |
| 24:AY:252:ASP:O     | 24:AY:254:LYS:HE3  | 1.93                     | 0.68              |
| 24:AY:491:VAL:HG11  | 24:AY:596:LYS:HD3  | 1.75                     | 0.68              |
| 27:B2:66:GLU:O      | 27:B2:69:ARG:HG2   | 1.93                     | 0.68              |
| 35:BA:1378:A:H4'    | 35:BA:1379:A:OP1   | 1.92                     | 0.68              |
| 35:BA:2393:A:H5''   | 48:BP:62:LEU:HB3   | 1.73                     | 0.68              |
| 42:BH:67:LEU:O      | 42:BH:71:LEU:HD12  | 1.93                     | 0.68              |
| 49:BQ:35:VAL:HG23   | 49:BQ:101:ARG:O    | 1.92                     | 0.68              |
| 50:BR:72:ASP:OD1    | 50:BR:75:LEU:HB2   | 1.93                     | 0.68              |
| 52:BT:75:ILE:N      | 52:BT:75:ILE:HD12  | 2.08                     | 0.68              |
| 9:CI:104:ARG:O      | 9:CI:105:ASP:HB3   | 1.92                     | 0.68              |
| 9:CI:48:GLU:N       | 9:CI:49:PRO:HD2    | 2.09                     | 0.68              |
| 11:CK:122:LYS:O     | 11:CK:124:LYS:N    | 2.26                     | 0.68              |
| 40:DF:53:THR:HG22   | 40:DF:56:GLU:CG    | 2.17                     | 0.68              |
| 50:DR:55:ALA:HA     | 50:DR:80:PHE:CE2   | 2.29                     | 0.68              |
| 1:AA:1404:C:H1'     | 1:AA:1499:A:C2     | 2.28                     | 0.68              |
| 5:AE:7:GLU:HG2      | 5:AE:112:LEU:HD22  | 1.74                     | 0.68              |
| 32:B7:6:GLN:O       | 35:BA:686:G:H1'    | 1.92                     | 0.68              |
| 35:BA:1120:G:H2'    | 35:BA:1121:C:C6    | 2.28                     | 0.68              |
| 35:BA:2122:U:H2'    | 35:BA:2123:G:H8    | 1.57                     | 0.68              |
| 35:BA:2068:U:N3     | 35:BA:2430:A:C2    | 2.61                     | 0.68              |
| 38:BD:61:LEU:O      | 38:BD:63:ARG:NH1   | 2.26                     | 0.68              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:BS:17:ARG:O     | 51:BS:20:ARG:HG2   | 1.92                     | 0.68              |
| 52:BT:57:PHE:O     | 52:BT:59:THR:HG23  | 1.92                     | 0.68              |
| 24:CY:316:ILE:HD12 | 24:CY:326:THR:HG22 | 1.74                     | 0.68              |
| 24:CY:91:THR:O     | 24:CY:93:GLU:N     | 2.26                     | 0.68              |
| 31:D6:30:THR:O     | 31:D6:32:ASN:N     | 2.26                     | 0.68              |
| 31:D6:37:ARG:NH2   | 35:DA:2286:A:H62   | 1.90                     | 0.68              |
| 42:DH:43:VAL:HG11  | 42:DH:52:VAL:HA    | 1.75                     | 0.68              |
| 48:DP:101:VAL:HG12 | 48:DP:106:LEU:HB3  | 1.75                     | 0.68              |
| 3:AC:123:GLN:HB3   | 3:AC:128:PHE:HD2   | 1.57                     | 0.68              |
| 12:AL:70:ILE:HD12  | 12:AL:75:HIS:CD2   | 2.28                     | 0.68              |
| 24:AY:343:ASN:HD21 | 24:AY:345:THR:HB   | 1.57                     | 0.68              |
| 31:B6:15:GLU:HG3   | 31:B6:47:THR:HG21  | 1.76                     | 0.68              |
| 35:BA:1053:C:C2'   | 35:BA:1054:A:H5''  | 2.24                     | 0.68              |
| 35:BA:1099:G:H2'   | 35:BA:1100:C:O4'   | 1.94                     | 0.68              |
| 35:BA:1779:U:C5    | 35:BA:1784:A:N7    | 2.61                     | 0.68              |
| 35:BA:2464:C:HO2'  | 35:BA:2465:C:H6    | 1.41                     | 0.68              |
| 35:BA:654:A:N7     | 35:BA:654(V):A:H4' | 2.08                     | 0.68              |
| 41:BG:173:LEU:HA   | 41:BG:176:LEU:HD12 | 1.74                     | 0.68              |
| 41:BG:57:ALA:O     | 41:BG:68:PRO:HG2   | 1.93                     | 0.68              |
| 35:BA:624:C:H41    | 48:BP:107:LYS:NZ   | 1.91                     | 0.68              |
| 51:BS:28:VAL:HG12  | 51:BS:29:PHE:N     | 2.07                     | 0.68              |
| 54:BV:19:LYS:HG2   | 54:BV:94:LEU:HB2   | 1.76                     | 0.68              |
| 57:BY:81:LYS:HD3   | 57:BY:97:ARG:O     | 1.92                     | 0.68              |
| 1:CA:474:G:H2'     | 1:CA:475:G:H8      | 1.58                     | 0.68              |
| 1:CA:793:U:C3'     | 1:CA:794:A:H5''    | 2.19                     | 0.68              |
| 5:CE:91:LEU:HD13   | 5:CE:120:THR:CG2   | 2.24                     | 0.68              |
| 33:D8:23:VAL:HG12  | 33:D8:46:ARG:HH11  | 1.57                     | 0.68              |
| 35:DA:1223:G:C3'   | 35:DA:1224:C:H5''  | 2.23                     | 0.68              |
| 31:D6:37:ARG:HH22  | 35:DA:2286:A:H62   | 1.41                     | 0.68              |
| 35:DA:389:G:H1     | 48:DP:71:VAL:HG12  | 1.58                     | 0.68              |
| 35:DA:733:G:H8     | 35:DA:733:G:O5'    | 1.75                     | 0.68              |
| 35:DA:940:G:H3'    | 35:DA:941:A:H5''   | 1.75                     | 0.68              |
| 38:DD:176:ARG:HH11 | 38:DD:176:ARG:HG2  | 1.58                     | 0.68              |
| 40:DF:154:VAL:HG11 | 40:DF:193:VAL:HG23 | 1.76                     | 0.68              |
| 52:DT:24:PRO:HD3   | 52:DT:52:ILE:CD1   | 2.24                     | 0.68              |
| 52:DT:85:LYS:HZ3   | 52:DT:85:LYS:HB3   | 1.59                     | 0.68              |
| 53:DU:20:LEU:H     | 53:DU:20:LEU:CD2   | 2.06                     | 0.68              |
| 57:DY:84:ARG:HG2   | 57:DY:84:ARG:HH11  | 1.59                     | 0.68              |
| 58:DZ:81:ARG:CZ    | 58:DZ:81:ARG:HB3   | 2.23                     | 0.68              |
| 2:AB:118:LEU:CB    | 2:AB:142:LEU:HD12  | 2.23                     | 0.68              |
| 4:AD:98:GLU:CG     | 4:AD:189:PRO:HG3   | 2.24                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:AJ:33:GLN:O     | 10:AJ:75:ILE:HG12  | 1.94                     | 0.68              |
| 26:B1:80:LEU:CD2   | 26:B1:81:LYS:H     | 2.04                     | 0.68              |
| 28:B3:28:LEU:HA    | 28:B3:33:GLN:OE1   | 1.94                     | 0.68              |
| 35:BA:1242:A:N1    | 48:BP:8:PRO:HG2    | 2.08                     | 0.68              |
| 35:BA:2761:G:C3'   | 35:BA:2762:G:H5''  | 2.22                     | 0.68              |
| 35:BA:900:A:H5'    | 35:BA:900:A:H8     | 1.59                     | 0.68              |
| 38:BD:261:LYS:HZ2  | 38:BD:263:ARG:HH12 | 1.39                     | 0.68              |
| 41:BG:34:LEU:HD11  | 41:BG:100:TRP:CH2  | 2.28                     | 0.68              |
| 41:BG:116:ASP:O    | 41:BG:117:PHE:HB3  | 1.94                     | 0.68              |
| 41:BG:131:TYR:HB3  | 41:BG:159:VAL:CG1  | 2.24                     | 0.68              |
| 42:BH:85:LYS:HZ3   | 42:BH:87:LEU:HG    | 1.56                     | 0.68              |
| 46:BN:65:LYS:HB3   | 46:BN:65:LYS:HZ2   | 1.58                     | 0.68              |
| 54:BV:6:LYS:O      | 54:BV:37:VAL:HG21  | 1.94                     | 0.68              |
| 2:CB:88:ALA:HB2    | 2:CB:219:VAL:HG13  | 1.74                     | 0.68              |
| 10:CJ:92:THR:HG23  | 10:CJ:93:GLY:H     | 1.57                     | 0.68              |
| 11:CK:59:TYR:CE2   | 11:CK:63:LEU:HD11  | 2.28                     | 0.68              |
| 12:CL:34:ARG:O     | 12:CL:61:THR:HG23  | 1.93                     | 0.68              |
| 12:CL:75:HIS:HD2   | 12:CL:77:LEU:HD12  | 1.59                     | 0.68              |
| 1:CA:1329:A:P      | 13:CM:28:ALA:HB3   | 2.33                     | 0.68              |
| 24:CY:114:VAL:O    | 24:CY:114:VAL:HG13 | 1.94                     | 0.68              |
| 24:CY:238:THR:HG22 | 24:CY:241:GLU:HG2  | 1.74                     | 0.68              |
| 29:D4:2:LYS:HB2    | 36:DB:40:U:O4      | 1.93                     | 0.68              |
| 35:DA:2262:U:C2'   | 35:DA:2263:C:H5'   | 2.24                     | 0.68              |
| 35:DA:2307:G:N2    | 35:DA:2308:G:H5''  | 2.07                     | 0.68              |
| 38:DD:71:ASP:HB2   | 38:DD:103:ARG:NH2  | 2.01                     | 0.68              |
| 38:DD:76:PRO:HG2   | 38:DD:98:VAL:HG21  | 1.76                     | 0.68              |
| 39:DE:179:GLU:HB3  | 39:DE:181:LEU:HD23 | 1.74                     | 0.68              |
| 50:DR:7:GLY:O      | 50:DR:8:ARG:HB2    | 1.92                     | 0.68              |
| 57:DY:27:VAL:HG12  | 57:DY:29:GLU:H     | 1.59                     | 0.68              |
| 1:AA:1298:C:H2'    | 1:AA:1298:C:O2     | 1.92                     | 0.68              |
| 2:AB:19:HIS:O      | 2:AB:20:GLU:O      | 2.12                     | 0.68              |
| 6:AF:16:GLN:CD     | 6:AF:16:GLN:N      | 2.47                     | 0.68              |
| 8:AH:42:GLU:HG3    | 8:AH:109:ILE:HD12  | 1.74                     | 0.68              |
| 11:AK:23:ALA:HB1   | 11:AK:88:GLY:HA3   | 1.76                     | 0.68              |
| 22:AV:3:C:H2'      | 22:AV:4:G:H5'      | 1.76                     | 0.68              |
| 27:B2:38:GLN:O     | 27:B2:41:ILE:HG12  | 1.93                     | 0.68              |
| 35:BA:272(I):U:O2  | 35:BA:272(I):U:H3' | 1.93                     | 0.68              |
| 35:BA:2807:G:C3'   | 35:BA:2808:U:H5''  | 2.23                     | 0.68              |
| 39:BE:170:LEU:HD12 | 39:BE:170:LEU:H    | 1.58                     | 0.68              |
| 1:CA:176:C:H2'     | 1:CA:177:C:H6      | 1.59                     | 0.68              |
| 3:CC:137:ALA:HA    | 3:CC:140:ARG:NH2   | 2.08                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:CD:10:ARG:O      | 4:CD:13:ARG:HB2    | 1.93                     | 0.68              |
| 24:CY:339:SER:HB2  | 24:CY:352:VAL:CG1  | 2.24                     | 0.68              |
| 27:D2:2:LYS:O      | 27:D2:6:VAL:HG23   | 1.94                     | 0.68              |
| 35:DA:528:A:C2     | 35:DA:2043:C:H4'   | 2.28                     | 0.68              |
| 35:DA:528:A:H2     | 35:DA:2043:C:H4'   | 1.57                     | 0.68              |
| 40:DF:178:PRO:HG2  | 40:DF:179:GLU:OE1  | 1.93                     | 0.68              |
| 47:DO:2:ILE:HD11   | 47:DO:82:ASN:HD22  | 1.59                     | 0.68              |
| 35:DA:2393:A:H5''  | 48:DP:62:LEU:HB3   | 1.76                     | 0.68              |
| 52:DT:45:PHE:CE2   | 52:DT:74:ARG:HB2   | 2.28                     | 0.68              |
| 52:DT:75:ILE:HD12  | 52:DT:75:ILE:N     | 2.09                     | 0.68              |
| 58:DZ:132:ASN:O    | 58:DZ:133:ILE:HD13 | 1.92                     | 0.68              |
| 1:AA:1234:C:O2'    | 1:AA:1235:U:H5'    | 1.94                     | 0.68              |
| 1:AA:376:G:H2'     | 1:AA:377:G:H8      | 1.59                     | 0.68              |
| 3:AC:34:LEU:HD22   | 3:AC:38:ARG:HD2    | 1.74                     | 0.68              |
| 16:AP:8:ARG:HB3    | 16:AP:28:ARG:NH1   | 2.09                     | 0.68              |
| 22:AV:17:C:H6      | 22:AV:17(A):U:C5   | 2.11                     | 0.68              |
| 24:AY:121:VAL:HG23 | 24:AY:122:TRP:N    | 2.09                     | 0.68              |
| 35:BA:1542:A:H5'   | 35:BA:1543:C:OP2   | 1.93                     | 0.68              |
| 35:BA:1656:C:H2'   | 35:BA:1657:C:H6    | 1.58                     | 0.68              |
| 35:BA:191:A:H2'    | 35:BA:192:C:C6     | 2.29                     | 0.68              |
| 30:B5:4:HIS:O      | 35:BA:2056:G:N2    | 2.26                     | 0.68              |
| 35:BA:2307:G:N2    | 35:BA:2308:G:H5''  | 2.08                     | 0.68              |
| 35:BA:2555:U:H2'   | 35:BA:2556:C:H5'   | 1.76                     | 0.68              |
| 35:BA:279:C:C2'    | 35:BA:280:C:H5''   | 2.24                     | 0.68              |
| 57:BY:84:ARG:HH11  | 57:BY:84:ARG:HG2   | 1.58                     | 0.68              |
| 58:BZ:150:LEU:N    | 58:BZ:150:LEU:HD23 | 2.09                     | 0.68              |
| 1:CA:1478:C:H2'    | 1:CA:1479:C:C6     | 2.28                     | 0.68              |
| 1:CA:183:G:H2'     | 1:CA:184:G:C8      | 2.29                     | 0.68              |
| 2:CB:223:ILE:HA    | 2:CB:226:ARG:NE    | 2.08                     | 0.68              |
| 3:CC:35:GLU:O      | 3:CC:38:ARG:HG2    | 1.92                     | 0.68              |
| 4:CD:162:LEU:HD11  | 4:CD:181:MET:HG2   | 1.75                     | 0.68              |
| 12:CL:113:ARG:HD2  | 12:CL:115:LYS:H    | 1.58                     | 0.68              |
| 13:CM:37:THR:HG21  | 13:CM:56:LEU:HD22  | 1.75                     | 0.68              |
| 18:CR:87:ARG:NH1   | 18:CR:87:ARG:HB3   | 2.09                     | 0.68              |
| 24:CY:265:LYS:O    | 24:CY:267:LYS:HG3  | 1.93                     | 0.68              |
| 24:CY:381:LYS:N    | 24:CY:381:LYS:HD2  | 2.07                     | 0.68              |
| 61:CY:702:FUA:O1   | 61:CY:702:FUA:H12  | 1.93                     | 0.68              |
| 35:DA:191:A:H2'    | 35:DA:192:C:C6     | 2.29                     | 0.68              |
| 35:DA:2039:C:H2'   | 35:DA:2040:C:C6    | 2.29                     | 0.68              |
| 35:DA:2631:G:N2    | 39:DE:61:ARG:HH12  | 1.91                     | 0.68              |
| 35:DA:548:A:C2'    | 35:DA:549:G:H5'    | 2.24                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:654(M):C:O2' | 35:DA:654(N):G:H8  | 1.77                     | 0.68              |
| 41:DG:141:PHE:HB2  | 41:DG:144:ILE:HG22 | 1.74                     | 0.68              |
| 42:DH:67:LEU:O     | 42:DH:71:LEU:HD12  | 1.94                     | 0.68              |
| 42:DH:86:GLU:CB    | 42:DH:132:ARG:HB3  | 2.24                     | 0.68              |
| 46:DN:21:LYS:HB3   | 46:DN:26:LEU:HD23  | 1.76                     | 0.68              |
| 48:DP:23:PRO:HB2   | 48:DP:33:ARG:CG    | 2.23                     | 0.68              |
| 50:DR:30:THR:OG1   | 50:DR:75:LEU:HD21  | 1.93                     | 0.68              |
| 1:AA:1014:A:H4'    | 19:AS:14:HIS:ND1   | 2.09                     | 0.68              |
| 1:AA:1442:G:H1     | 1:AA:1461:G:H21    | 1.42                     | 0.68              |
| 1:AA:1104:G:O5'    | 2:AB:111:ARG:HD2   | 1.93                     | 0.68              |
| 13:AM:15:VAL:O     | 13:AM:19:LEU:HD23  | 1.94                     | 0.68              |
| 22:AV:61:C:O2'     | 22:AV:62:C:H5'     | 1.94                     | 0.68              |
| 23:AX:19:U:C5'     | 24:AY:504:ARG:HB3  | 2.23                     | 0.68              |
| 30:B5:44:THR:HG22  | 30:B5:45:VAL:N     | 2.08                     | 0.68              |
| 35:BA:1058:G:N2    | 35:BA:1081:U:H1'   | 2.08                     | 0.68              |
| 35:BA:1697:G:H3'   | 35:BA:1698:A:H5''  | 1.74                     | 0.68              |
| 35:BA:85:G:OP1     | 57:BY:30:VAL:HB    | 1.93                     | 0.68              |
| 41:BG:42:GLY:O     | 41:BG:44:GLY:N     | 2.25                     | 0.68              |
| 42:BH:37:VAL:HG12  | 42:BH:38:SER:N     | 2.09                     | 0.68              |
| 50:BR:55:ALA:HA    | 50:BR:80:PHE:CE2   | 2.29                     | 0.68              |
| 57:BY:31:LEU:HD22  | 57:BY:31:LEU:N     | 2.09                     | 0.68              |
| 1:CA:1358:U:OP1    | 14:CN:35:ARG:HG3   | 1.94                     | 0.68              |
| 5:CE:7:GLU:HG2     | 5:CE:112:LEU:CD2   | 2.23                     | 0.68              |
| 16:CP:60:LEU:HA    | 16:CP:64:ALA:HB3   | 1.76                     | 0.68              |
| 24:CY:424:LEU:HD12 | 24:CY:427:ALA:HB3  | 1.76                     | 0.68              |
| 24:CY:84:THR:HA    | 61:CY:702:FUA:C32  | 2.21                     | 0.68              |
| 35:DA:1541:G:H4'   | 35:DA:1542:A:C5'   | 2.24                     | 0.68              |
| 35:DA:1599:C:H2'   | 35:DA:1600:C:H6    | 1.58                     | 0.68              |
| 35:DA:2105:C:H42   | 35:DA:2184:G:H1    | 1.41                     | 0.68              |
| 35:DA:756:C:O2'    | 35:DA:757:U:H5'    | 1.94                     | 0.68              |
| 37:DC:28:ARG:HG2   | 37:DC:183:PRO:HB3  | 1.76                     | 0.68              |
| 46:DN:55:VAL:HG22  | 46:DN:126:PRO:HA   | 1.75                     | 0.68              |
| 48:DP:58:THR:O     | 48:DP:61:ARG:NE    | 2.19                     | 0.68              |
| 48:DP:79:ARG:O     | 48:DP:111:ARG:HB2  | 1.93                     | 0.68              |
| 48:DP:84:ASN:HA    | 48:DP:115:LEU:O    | 1.93                     | 0.68              |
| 51:DS:70:GLY:C     | 51:DS:101:LEU:HD23 | 2.14                     | 0.68              |
| 5:AE:101:ILE:HD13  | 5:AE:118:ILE:O     | 1.94                     | 0.68              |
| 19:AS:58:VAL:HG23  | 19:AS:58:VAL:O     | 1.93                     | 0.68              |
| 24:AY:367:GLU:HG2  | 24:AY:367:GLU:O    | 1.94                     | 0.68              |
| 26:B1:84:GLY:O     | 26:B1:86:SER:N     | 2.27                     | 0.68              |
| 35:BA:606:U:H2'    | 35:BA:606:U:O2     | 1.93                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 39:BE:48:GLN:HE21 | 39:BE:78:LEU:HD22  | 1.59                     | 0.68              |
| 42:BH:86:GLU:CB   | 42:BH:132:ARG:HB3  | 2.24                     | 0.68              |
| 46:BN:3:THR:HG22  | 46:BN:4:TYR:N      | 2.09                     | 0.68              |
| 53:BU:107:ALA:HA  | 53:BU:110:VAL:CG2  | 2.24                     | 0.68              |
| 1:CA:1324:A:H2'   | 1:CA:1325:C:C6     | 2.28                     | 0.68              |
| 1:CA:793:U:H3'    | 1:CA:794:A:C5'     | 2.21                     | 0.68              |
| 4:CD:24:GLU:O     | 4:CD:27:TYR:HB2    | 1.94                     | 0.68              |
| 21:CU:2:GLY:O     | 21:CU:4:GLY:N      | 2.26                     | 0.68              |
| 24:CY:238:THR:C   | 24:CY:240:GLU:H    | 1.97                     | 0.68              |
| 24:CY:487:ILE:HB  | 24:CY:597:GLY:O    | 1.94                     | 0.68              |
| 26:D1:30:VAL:HG23 | 26:D1:31:GLY:N     | 2.08                     | 0.68              |
| 31:D6:11:LEU:HG   | 31:D6:26:ASN:ND2   | 2.09                     | 0.68              |
| 35:DA:2720:U:H2'  | 35:DA:2721:A:H8    | 1.57                     | 0.68              |
| 35:DA:612:C:H2'   | 35:DA:613:G:C5'    | 2.13                     | 0.68              |
| 35:DA:900:A:H5'   | 35:DA:900:A:H8     | 1.59                     | 0.68              |
| 40:DF:4:VAL:HG13  | 40:DF:19:GLU:OE2   | 1.93                     | 0.68              |
| 41:DG:98:ARG:HH11 | 41:DG:98:ARG:HG2   | 1.59                     | 0.68              |
| 35:DA:631:A:OP1   | 48:DP:64:LYS:HE2   | 1.94                     | 0.68              |
| 48:DP:7:ARG:CB    | 48:DP:8:PRO:HD3    | 2.23                     | 0.68              |
| 58:DZ:7:ALA:CB    | 58:DZ:61:LEU:HD23  | 2.23                     | 0.68              |
| 3:AC:82:GLU:O     | 3:AC:86:VAL:HG13   | 1.93                     | 0.68              |
| 11:AK:108:ILE:N   | 11:AK:108:ILE:HD12 | 2.08                     | 0.68              |
| 24:AY:21:ILE:O    | 24:AY:22:ASP:HB2   | 1.93                     | 0.68              |
| 24:AY:309:LEU:O   | 24:AY:390:VAL:HA   | 1.93                     | 0.68              |
| 24:AY:39:ILE:HG23 | 24:AY:41:LYS:HE3   | 1.75                     | 0.68              |
| 25:B0:7:LEU:CD1   | 49:BQ:85:LYS:HE2   | 2.22                     | 0.68              |
| 26:B1:82:LEU:O    | 26:B1:83:GLU:HG3   | 1.94                     | 0.68              |
| 35:BA:2720:U:H2'  | 35:BA:2721:A:H8    | 1.57                     | 0.68              |
| 40:BF:107:LYS:O   | 40:BF:110:LEU:N    | 2.27                     | 0.68              |
| 48:BP:23:PRO:HB2  | 48:BP:33:ARG:CG    | 2.24                     | 0.68              |
| 52:BT:129:ARG:HG2 | 52:BT:129:ARG:O    | 1.92                     | 0.68              |
| 1:CA:332:G:H2'    | 1:CA:333:G:H8      | 1.60                     | 0.68              |
| 1:CA:376:G:H2'    | 1:CA:377:G:H8      | 1.59                     | 0.68              |
| 4:CD:57:ARG:HB3   | 4:CD:206:PHE:HB2   | 1.76                     | 0.68              |
| 11:CK:84:VAL:HG11 | 11:CK:95:ILE:HD11  | 1.76                     | 0.68              |
| 1:CA:1358:U:P     | 14:CN:35:ARG:HG3   | 2.34                     | 0.68              |
| 30:D5:44:THR:HG22 | 30:D5:45:VAL:N     | 2.09                     | 0.68              |
| 31:D6:15:GLU:HG3  | 31:D6:47:THR:HG21  | 1.75                     | 0.68              |
| 35:DA:1395:A:H4'  | 35:DA:1397:U:C5    | 2.29                     | 0.68              |
| 35:DA:1697:G:H3'  | 35:DA:1698:A:H5''  | 1.75                     | 0.68              |
| 35:DA:2074:U:H2'  | 35:DA:2075:U:C6    | 2.29                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:2476:A:N1    | 35:DA:2477:C:C5    | 2.62                     | 0.68              |
| 35:DA:739:G:H4'    | 35:DA:740:U:OP1    | 1.94                     | 0.68              |
| 39:DE:170:LEU:H    | 39:DE:170:LEU:HD12 | 1.60                     | 0.68              |
| 35:DA:2308:G:N2    | 41:DG:79:ASN:HB2   | 2.09                     | 0.68              |
| 48:DP:13:ASN:O     | 48:DP:14:LYS:HB2   | 1.93                     | 0.68              |
| 53:DU:112:ARG:NH2  | 54:DV:46:VAL:HG11  | 2.08                     | 0.68              |
| 1:AA:1231:G:O2'    | 1:AA:1232:U:H5'    | 1.94                     | 0.67              |
| 1:AA:1308:U:H5''   | 13:AM:98:VAL:HG23  | 1.77                     | 0.67              |
| 1:AA:267:C:H2'     | 1:AA:268:C:H6      | 1.59                     | 0.67              |
| 2:AB:233:SER:HB2   | 2:AB:234:PRO:CD    | 2.24                     | 0.67              |
| 24:AY:335:LEU:HD11 | 24:AY:352:VAL:HG11 | 1.73                     | 0.67              |
| 25:B0:51:VAL:HG22  | 25:B0:81:VAL:HG23  | 1.74                     | 0.67              |
| 35:BA:1865:G:H2'   | 35:BA:1866:C:H5''  | 1.76                     | 0.67              |
| 35:BA:1567:A:H2'   | 38:BD:84:TYR:HE2   | 1.59                     | 0.67              |
| 51:BS:95:HIS:CG    | 51:BS:96:GLY:N     | 2.61                     | 0.67              |
| 52:BT:107:ASP:CG   | 52:BT:108:ARG:H    | 1.96                     | 0.67              |
| 52:BT:115:ARG:CB   | 52:BT:115:ARG:HH11 | 2.03                     | 0.67              |
| 1:CA:267:C:H2'     | 1:CA:268:C:H6      | 1.58                     | 0.67              |
| 1:CA:160:A:H1'     | 1:CA:344:A:C5      | 2.29                     | 0.67              |
| 22:CV:47:U:H3'     | 22:CV:48:C:C5'     | 2.22                     | 0.67              |
| 24:CY:467:LYS:O    | 24:CY:471:LYS:HA   | 1.94                     | 0.67              |
| 26:D1:56:GLN:NE2   | 26:D1:87:PRO:HB3   | 2.08                     | 0.67              |
| 28:D3:28:LEU:HA    | 28:D3:33:GLN:OE1   | 1.93                     | 0.67              |
| 33:D8:52:LYS:N     | 33:D8:53:PRO:CD    | 2.56                     | 0.67              |
| 35:DA:142:A:H5'    | 35:DA:142(A):C:OP2 | 1.94                     | 0.67              |
| 35:DA:1538:G:H2'   | 35:DA:1539:G:H8    | 1.59                     | 0.67              |
| 35:DA:1831:G:H2'   | 35:DA:1832:C:C6    | 2.29                     | 0.67              |
| 35:DA:555:U:H2'    | 35:DA:556:G:C8     | 2.29                     | 0.67              |
| 32:D7:6:GLN:O      | 35:DA:686:G:H1'    | 1.94                     | 0.67              |
| 40:DF:167:ALA:HB1  | 40:DF:173:VAL:CG1  | 2.21                     | 0.67              |
| 42:DH:124:GLU:HB2  | 42:DH:132:ARG:HG3  | 1.77                     | 0.67              |
| 42:DH:154:PRO:O    | 42:DH:156:ALA:N    | 2.25                     | 0.67              |
| 49:DQ:27:VAL:HG23  | 49:DQ:137:TYR:CD2  | 2.30                     | 0.67              |
| 53:DU:68:ALA:O     | 53:DU:71:GLN:HB3   | 1.93                     | 0.67              |
| 1:AA:332:G:H2'     | 1:AA:333:G:H8      | 1.58                     | 0.67              |
| 3:AC:35:GLU:O      | 3:AC:38:ARG:HG2    | 1.94                     | 0.67              |
| 4:AD:13:ARG:HA     | 4:AD:33:MET:CE     | 2.24                     | 0.67              |
| 10:AJ:13:HIS:O     | 10:AJ:17:ASP:HB2   | 1.94                     | 0.67              |
| 1:AA:522:C:H41     | 12:AL:53:ARG:HH22  | 1.41                     | 0.67              |
| 25:B0:20:ARG:HD2   | 25:B0:20:ARG:H     | 1.56                     | 0.67              |
| 35:BA:566:U:O2'    | 35:BA:567:A:H5'    | 1.93                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 35:BA:769:G:O2'     | 35:BA:770:G:H5'    | 1.94                     | 0.67              |
| 37:BC:4:HIS:ND1     | 37:BC:8:TYR:HE2    | 1.92                     | 0.67              |
| 39:BE:63:LEU:O      | 39:BE:63:LEU:HD23  | 1.93                     | 0.67              |
| 41:BG:106:LEU:HA    | 41:BG:110:ALA:CB   | 2.23                     | 0.67              |
| 46:BN:58:ASP:O      | 46:BN:60:ILE:N     | 2.27                     | 0.67              |
| 50:BR:63:ARG:NH2    | 50:BR:77:ARG:HG2   | 2.08                     | 0.67              |
| 52:BT:129:ARG:O     | 52:BT:131:ALA:N    | 2.22                     | 0.67              |
| 35:BA:518:G:H4'     | 55:BW:18:ARG:NH1   | 2.09                     | 0.67              |
| 58:BZ:156:LYS:O     | 58:BZ:158:PRO:HD3  | 1.94                     | 0.67              |
| 4:CD:88:VAL:O       | 4:CD:92:VAL:HG23   | 1.95                     | 0.67              |
| 7:CG:102:ARG:HG2    | 7:CG:106:GLN:NE2   | 2.09                     | 0.67              |
| 10:CJ:61:GLU:OE2    | 14:CN:45:ARG:HD2   | 1.94                     | 0.67              |
| 12:CL:17:LYS:HD3    | 12:CL:18:VAL:HG22  | 1.74                     | 0.67              |
| 24:CY:454:MET:H     | 24:CY:458:HIS:HD2  | 1.41                     | 0.67              |
| 35:DA:2712:U:HO2'   | 35:DA:2712(A):A:H8 | 0.74                     | 0.67              |
| 35:DA:2713:A:H3'    | 35:DA:2714:G:C5'   | 2.25                     | 0.67              |
| 35:DA:654:A:N7      | 35:DA:654(V):A:H4' | 2.09                     | 0.67              |
| 35:DA:2591:C:OP2    | 38:DD:239:ARG:HB3  | 1.94                     | 0.67              |
| 38:DD:39:LYS:NZ     | 38:DD:87:ASN:HB3   | 2.09                     | 0.67              |
| 48:DP:23:PRO:HB2    | 48:DP:33:ARG:CD    | 2.24                     | 0.67              |
| 51:DS:66:ALA:O      | 51:DS:99:LYS:HA    | 1.94                     | 0.67              |
| 52:DT:55:ASN:H      | 52:DT:59:THR:CG2   | 2.06                     | 0.67              |
| 53:DU:113:ALA:C     | 53:DU:115:ALA:H    | 1.98                     | 0.67              |
| 56:DX:30:VAL:HG22   | 56:DX:77:LYS:O     | 1.94                     | 0.67              |
| 1:AA:60:A:H5''      | 1:AA:331:G:H22     | 1.58                     | 0.67              |
| 1:AA:1190:G:OP1     | 3:AC:5:ILE:HD12    | 1.94                     | 0.67              |
| 12:AL:86:ARG:NH2    | 12:AL:99:HIS:CD2   | 2.63                     | 0.67              |
| 22:AW:1:C:H2'       | 22:AW:2:G:H8       | 1.59                     | 0.67              |
| 28:B3:28:LEU:N      | 28:B3:28:LEU:HD23  | 2.09                     | 0.67              |
| 28:B3:59:VAL:HG12   | 28:B3:60:GLU:N     | 2.09                     | 0.67              |
| 35:BA:1528(A):A:H62 | 35:BA:1541:G:N2    | 1.92                     | 0.67              |
| 35:BA:1639:U:O2'    | 35:BA:1640:C:H5''  | 1.94                     | 0.67              |
| 35:BA:1819:A:H4'    | 35:BA:1820:U:H5'   | 1.76                     | 0.67              |
| 35:BA:548:A:C2'     | 35:BA:549:G:H5'    | 2.24                     | 0.67              |
| 35:BA:555:U:H2'     | 35:BA:556:G:C8     | 2.29                     | 0.67              |
| 35:BA:581:C:H2'     | 35:BA:582:G:C8     | 2.29                     | 0.67              |
| 38:BD:267:SER:CA    | 38:BD:270:ILE:HD11 | 2.25                     | 0.67              |
| 40:BF:152:GLU:O     | 40:BF:154:VAL:HG23 | 1.94                     | 0.67              |
| 53:BU:55:ARG:HA     | 53:BU:58:ARG:CG    | 2.24                     | 0.67              |
| 1:CA:1161:C:H2'     | 1:CA:1162:C:H6     | 1.58                     | 0.67              |
| 1:CA:473:G:H2'      | 1:CA:474:G:H8      | 1.59                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:CY:388:THR:CG2 | 24:CY:399:LEU:HD13 | 2.24                     | 0.67              |
| 24:CY:65:ILE:O    | 24:CY:67:ALA:N     | 2.26                     | 0.67              |
| 30:D5:25:LEU:CD1  | 55:DW:19:LEU:HB3   | 2.25                     | 0.67              |
| 34:D9:17:ILE:HG21 | 34:D9:19:ARG:HH21  | 1.60                     | 0.67              |
| 35:DA:1718:G:H5'  | 35:DA:1718:G:H8    | 1.60                     | 0.67              |
| 27:D2:46:GLN:OE1  | 35:DA:95:G:H4'     | 1.94                     | 0.67              |
| 35:DA:970:C:H2'   | 35:DA:971:C:C6     | 2.29                     | 0.67              |
| 38:DD:183:ARG:HG2 | 38:DD:183:ARG:NH1  | 2.08                     | 0.67              |
| 40:DF:43:LYS:HA   | 40:DF:98:SER:HB3   | 1.74                     | 0.67              |
| 41:DG:60:LEU:O    | 41:DG:63:ILE:HG13  | 1.93                     | 0.67              |
| 51:DS:85:VAL:HG23 | 51:DS:106:ARG:HG3  | 1.76                     | 0.67              |
| 51:DS:28:VAL:HG12 | 51:DS:29:PHE:N     | 2.07                     | 0.67              |
| 57:DY:31:LEU:HD22 | 57:DY:31:LEU:N     | 2.08                     | 0.67              |
| 2:AB:167:PRO:HG2  | 2:AB:192:SER:OG    | 1.94                     | 0.67              |
| 3:AC:150:LYS:HB2  | 3:AC:169:ALA:HB1   | 1.76                     | 0.67              |
| 5:AE:36:ASP:OD2   | 5:AE:40:ARG:HB2    | 1.93                     | 0.67              |
| 9:AI:48:GLU:N     | 9:AI:49:PRO:HD2    | 2.10                     | 0.67              |
| 9:AI:4:TYR:CD2    | 9:AI:88:TYR:HB2    | 2.29                     | 0.67              |
| 12:AL:113:ARG:HD2 | 12:AL:115:LYS:H    | 1.58                     | 0.67              |
| 25:B0:16:SER:HB2  | 35:BA:2262:U:H5    | 1.59                     | 0.67              |
| 29:B4:1:MET:HG2   | 41:BG:98:ARG:NE    | 2.09                     | 0.67              |
| 30:B5:19:ARG:HA   | 35:BA:2046:G:H5'   | 1.76                     | 0.67              |
| 35:BA:20:C:O2'    | 35:BA:21:A:H5'     | 1.93                     | 0.67              |
| 35:BA:2346:A:H1'  | 35:BA:2383:G:C8    | 2.29                     | 0.67              |
| 35:BA:903:C:H2'   | 35:BA:904:C:C5'    | 2.18                     | 0.67              |
| 41:BG:173:LEU:HA  | 41:BG:176:LEU:CD1  | 2.25                     | 0.67              |
| 51:BS:89:ARG:O    | 51:BS:92:TYR:HB3   | 1.94                     | 0.67              |
| 2:CB:21:ARG:HD2   | 2:CB:39:ILE:HG12   | 1.74                     | 0.67              |
| 3:CC:123:GLN:HB3  | 3:CC:128:PHE:HD2   | 1.58                     | 0.67              |
| 4:CD:5:ILE:HA     | 4:CD:115:ARG:HH12  | 1.57                     | 0.67              |
| 19:CS:40:ILE:HG21 | 19:CS:66:MET:O     | 1.95                     | 0.67              |
| 20:CT:48:LYS:HB3  | 20:CT:51:GLU:HG2   | 1.77                     | 0.67              |
| 27:D2:32:LEU:HB2  | 27:D2:53:LEU:HD22  | 1.75                     | 0.67              |
| 35:DA:2329:G:H2'  | 35:DA:2330:G:C8    | 2.29                     | 0.67              |
| 35:DA:2466:C:O2'  | 35:DA:2467:C:H5'   | 1.94                     | 0.67              |
| 39:DE:78:LEU:O    | 39:DE:79:ARG:HD2   | 1.93                     | 0.67              |
| 50:DR:10:LEU:HD22 | 50:DR:17:ARG:HD3   | 1.76                     | 0.67              |
| 53:DU:83:LEU:H    | 53:DU:83:LEU:CD1   | 2.08                     | 0.67              |
| 58:DZ:153:SER:HB2 | 58:DZ:163:LEU:CD1  | 2.23                     | 0.67              |
| 1:AA:1456:G:C2'   | 1:AA:1457:G:H5'    | 2.24                     | 0.67              |
| 1:AA:584:G:H2'    | 1:AA:585:G:H8      | 1.59                     | 0.67              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:AP:49:LEU:HD22  | 16:AP:73:LEU:HD22  | 1.74                     | 0.67              |
| 35:BA:2524:G:C8    | 35:BA:2524:G:H5'   | 2.28                     | 0.67              |
| 39:BE:131:ALA:CB   | 39:BE:134:ILE:HD11 | 2.15                     | 0.67              |
| 41:BG:54:GLU:O     | 41:BG:57:ALA:HB3   | 1.94                     | 0.67              |
| 41:BG:61:ALA:HB1   | 41:BG:66:GLN:O     | 1.95                     | 0.67              |
| 46:BN:45:ASN:ND2   | 46:BN:45:ASN:H     | 1.90                     | 0.67              |
| 35:BA:807:U:OP2    | 48:BP:39:LYS:HG3   | 1.95                     | 0.67              |
| 51:BS:49:VAL:HG12  | 51:BS:50:SER:N     | 2.08                     | 0.67              |
| 54:BV:28:GLU:OE1   | 54:BV:31:ALA:HB2   | 1.94                     | 0.67              |
| 1:CA:1211:U:H5'    | 1:CA:1212:U:OP1    | 1.94                     | 0.67              |
| 24:CY:680:PRO:O    | 24:CY:682:GLN:HG2  | 1.93                     | 0.67              |
| 29:D4:14:ILE:N     | 29:D4:14:ILE:HD12  | 2.10                     | 0.67              |
| 35:DA:1030:G:OP2   | 49:DQ:128:LYS:HE2  | 1.95                     | 0.67              |
| 35:DA:364:C:C2'    | 35:DA:365:C:H5''   | 2.24                     | 0.67              |
| 39:DE:63:LEU:HD23  | 39:DE:63:LEU:O     | 1.93                     | 0.67              |
| 40:DF:107:LYS:O    | 40:DF:110:LEU:N    | 2.26                     | 0.67              |
| 48:DP:62:LEU:N     | 48:DP:62:LEU:CD2   | 2.58                     | 0.67              |
| 1:AA:1325:C:H2'    | 1:AA:1326:C:H6     | 1.58                     | 0.67              |
| 2:AB:204:ASN:C     | 2:AB:204:ASN:HD22  | 1.94                     | 0.67              |
| 3:AC:70:VAL:CG1    | 3:AC:71:ALA:H      | 2.06                     | 0.67              |
| 5:AE:155:GLU:N     | 8:AH:46:LYS:HG2    | 2.09                     | 0.67              |
| 24:AY:72:CYS:SG    | 24:AY:79:ILE:HB    | 2.34                     | 0.67              |
| 31:B6:10:LEU:H     | 31:B6:10:LEU:HD23  | 1.58                     | 0.67              |
| 33:B8:33:ASN:O     | 33:B8:34:TRP:HB3   | 1.93                     | 0.67              |
| 35:BA:1113:U:H2'   | 35:BA:1114:G:C8    | 2.29                     | 0.67              |
| 35:BA:1395:A:H4'   | 35:BA:1397:U:C5    | 2.30                     | 0.67              |
| 35:BA:363(B):G:H2' | 35:BA:363(C):G:H8  | 1.58                     | 0.67              |
| 35:BA:559:G:H22    | 53:BU:49:HIS:CD2   | 2.13                     | 0.67              |
| 40:BF:25:PRO:HG3   | 40:BF:119:ARG:HB2  | 1.76                     | 0.67              |
| 41:BG:82:LEU:HD11  | 41:BG:87:PRO:HB3   | 1.76                     | 0.67              |
| 46:BN:48:MET:CE    | 46:BN:48:MET:H     | 2.06                     | 0.67              |
| 49:BQ:27:VAL:HG23  | 49:BQ:137:TYR:CD2  | 2.29                     | 0.67              |
| 35:BA:958:U:OP2    | 49:BQ:14:ARG:NH1   | 2.27                     | 0.67              |
| 54:BV:39:LEU:O     | 54:BV:40:LEU:HB2   | 1.93                     | 0.67              |
| 55:BW:68:ARG:HA    | 55:BW:110:LYS:HG2  | 1.76                     | 0.67              |
| 1:CA:1459:C:H2'    | 1:CA:1460:A:C8     | 2.30                     | 0.67              |
| 2:CB:118:LEU:CB    | 2:CB:142:LEU:HD12  | 2.21                     | 0.67              |
| 12:CL:70:ILE:HD12  | 12:CL:75:HIS:CD2   | 2.29                     | 0.67              |
| 24:CY:293:THR:HB   | 24:CY:294:PRO:HD2  | 1.76                     | 0.67              |
| 31:D6:38:LYS:HD3   | 35:DA:2344:U:OP1   | 1.94                     | 0.67              |
| 35:DA:2593:U:H2'   | 35:DA:2594:C:C6    | 2.29                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:DF:132:VAL:HG22 | 40:DF:133:ASN:N    | 2.10                     | 0.67              |
| 40:DF:89:VAL:HG12  | 40:DF:90:PHE:N     | 2.09                     | 0.67              |
| 41:DG:121:ASN:HB3  | 41:DG:124:SER:CB   | 2.22                     | 0.67              |
| 48:DP:85:LEU:CD1   | 48:DP:120:ALA:HB2  | 2.22                     | 0.67              |
| 52:DT:23:ARG:HB2   | 52:DT:24:PRO:HD2   | 1.77                     | 0.67              |
| 54:DV:6:LYS:O      | 54:DV:37:VAL:HG21  | 1.94                     | 0.67              |
| 1:AA:1424:C:H2'    | 1:AA:1425:U:H6     | 1.60                     | 0.67              |
| 1:AA:973:G:H3'     | 1:AA:974:A:H5''    | 1.76                     | 0.67              |
| 2:AB:21:ARG:HD2    | 2:AB:39:ILE:HG12   | 1.75                     | 0.67              |
| 4:AD:33:MET:O      | 4:AD:37:PRO:HG3    | 1.94                     | 0.67              |
| 8:AH:103:VAL:CG2   | 8:AH:110:ALA:HB2   | 2.25                     | 0.67              |
| 10:AJ:4:ILE:HD12   | 10:AJ:4:ILE:N      | 2.09                     | 0.67              |
| 13:AM:37:THR:HG21  | 13:AM:56:LEU:HD22  | 1.76                     | 0.67              |
| 27:B2:21:LEU:O     | 27:B2:24:LEU:HB3   | 1.95                     | 0.67              |
| 35:BA:1790:C:H5''  | 35:BA:1791:A:OP1   | 1.95                     | 0.67              |
| 39:BE:113:PHE:CE2  | 39:BE:158:GLY:HA2  | 2.30                     | 0.67              |
| 39:BE:4:ILE:HD11   | 39:BE:28:ALA:HB1   | 1.77                     | 0.67              |
| 51:BS:74:ALA:HB1   | 51:BS:103:GLU:CB   | 2.24                     | 0.67              |
| 52:BT:82:LEU:N     | 52:BT:82:LEU:HD12  | 2.10                     | 0.67              |
| 53:BU:20:LEU:N     | 53:BU:20:LEU:HD22  | 2.08                     | 0.67              |
| 1:CA:584:G:H2'     | 1:CA:585:G:C8      | 2.30                     | 0.67              |
| 2:CB:233:SER:HB2   | 2:CB:234:PRO:CD    | 2.24                     | 0.67              |
| 2:CB:43:ASP:OD2    | 2:CB:46:LYS:HB2    | 1.95                     | 0.67              |
| 24:CY:82:ILE:HD12  | 24:CY:101:LEU:HD23 | 1.75                     | 0.67              |
| 24:CY:453:GLY:HA3  | 24:CY:459:LEU:HD23 | 1.77                     | 0.67              |
| 27:D2:58:ALA:HB1   | 35:DA:76:C:C4'     | 2.24                     | 0.67              |
| 33:D8:4:MET:O      | 33:D8:62:LEU:HD12  | 1.95                     | 0.67              |
| 35:DA:1504:C:H2'   | 35:DA:1505:C:H5''  | 1.75                     | 0.67              |
| 35:DA:2186:G:H2'   | 35:DA:2187:G:H5''  | 1.77                     | 0.67              |
| 35:DA:271(J):C:H2' | 35:DA:271(J):C:O2  | 1.94                     | 0.67              |
| 35:DA:2832:U:H1'   | 35:DA:2834:G:N3    | 2.10                     | 0.67              |
| 35:DA:813:U:H2'    | 35:DA:814:C:H6     | 1.59                     | 0.67              |
| 39:DE:117:MET:HG2  | 39:DE:117:MET:O    | 1.94                     | 0.67              |
| 40:DF:192:LEU:C    | 40:DF:192:LEU:HD23 | 2.15                     | 0.67              |
| 1:AA:1161:C:H2'    | 1:AA:1162:C:C6     | 2.29                     | 0.67              |
| 1:AA:160:A:H1'     | 1:AA:344:A:C5      | 2.29                     | 0.67              |
| 4:AD:5:ILE:HA      | 4:AD:115:ARG:HH12  | 1.60                     | 0.67              |
| 37:BC:78:ILE:O     | 37:BC:120:VAL:HG21 | 1.95                     | 0.67              |
| 38:BD:172:TYR:CD1  | 38:BD:186:HIS:HA   | 2.30                     | 0.67              |
| 46:BN:55:VAL:HG22  | 46:BN:126:PRO:HA   | 1.74                     | 0.67              |
| 46:BN:43:THR:O     | 46:BN:46:VAL:HG12  | 1.94                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:BQ:79:LEU:HD23  | 49:BQ:80:GLU:H     | 1.58                     | 0.67              |
| 51:BS:85:VAL:HG23  | 51:BS:106:ARG:HG3  | 1.76                     | 0.67              |
| 54:BV:18:LEU:HD13  | 54:BV:19:LYS:H     | 1.59                     | 0.67              |
| 2:CB:19:HIS:O      | 2:CB:20:GLU:O      | 2.12                     | 0.67              |
| 3:CC:134:ILE:HD11  | 3:CC:153:VAL:HG23  | 1.76                     | 0.67              |
| 10:CJ:32:ALA:HB2   | 10:CJ:76:ASN:ND2   | 2.10                     | 0.67              |
| 14:CN:12:ARG:C     | 14:CN:14:PRO:HD3   | 2.15                     | 0.67              |
| 17:CQ:47:PRO:HG2   | 17:CQ:48:GLU:OE2   | 1.94                     | 0.67              |
| 24:CY:137:ASN:HD21 | 24:CY:263:ALA:CB   | 2.08                     | 0.67              |
| 24:CY:631:ILE:HG21 | 35:DA:1067:A:C4    | 2.30                     | 0.67              |
| 35:DA:1435:G:H5'   | 35:DA:1436:G:OP2   | 1.93                     | 0.67              |
| 35:DA:581:C:H2'    | 35:DA:582:G:C8     | 2.29                     | 0.67              |
| 35:DA:825:C:O2'    | 35:DA:826:U:H5'    | 1.94                     | 0.67              |
| 35:DA:910:A:C5     | 49:DQ:13:GLN:HG3   | 2.30                     | 0.67              |
| 39:DE:4:ILE:HD11   | 39:DE:28:ALA:HB1   | 1.77                     | 0.67              |
| 35:DA:1081:U:H5''  | 44:DK:122:ALA:HB1  | 1.77                     | 0.67              |
| 52:DT:106:SER:HA   | 52:DT:110:ILE:HG12 | 1.77                     | 0.67              |
| 1:AA:1161:C:H2'    | 1:AA:1162:C:H6     | 1.60                     | 0.67              |
| 1:AA:176:C:H2'     | 1:AA:177:C:H6      | 1.59                     | 0.67              |
| 18:AR:87:ARG:NH1   | 18:AR:87:ARG:HB3   | 2.10                     | 0.67              |
| 20:AT:82:SER:O     | 20:AT:86:ARG:HB2   | 1.95                     | 0.67              |
| 21:AU:2:GLY:O      | 21:AU:4:GLY:N      | 2.28                     | 0.67              |
| 24:AY:395:PRO:O    | 24:AY:397:VAL:N    | 2.27                     | 0.67              |
| 35:BA:1367:A:H2'   | 35:BA:1368:G:H5'   | 1.75                     | 0.67              |
| 35:BA:419:C:H2'    | 35:BA:420:C:C6     | 2.29                     | 0.67              |
| 51:BS:30:ARG:HD3   | 51:BS:97:ARG:HG2   | 1.75                     | 0.67              |
| 1:CA:522:C:H41     | 12:CL:53:ARG:HH22  | 1.42                     | 0.67              |
| 4:CD:189:PRO:HB2   | 4:CD:194:LEU:HD21  | 1.76                     | 0.67              |
| 16:CP:74:LEU:CD2   | 16:CP:79:VAL:HG21  | 2.24                     | 0.67              |
| 22:CV:49:G:H1      | 22:CV:65:C:N4      | 1.92                     | 0.67              |
| 24:CY:145:ASP:O    | 24:CY:149:VAL:HG23 | 1.93                     | 0.67              |
| 24:CY:553:GLY:H    | 24:CY:557:GLY:HA2  | 1.60                     | 0.67              |
| 24:CY:655:TYR:OH   | 24:CY:659:LEU:HD23 | 1.95                     | 0.67              |
| 27:D2:2:LYS:CB     | 35:DA:97:C:H5''    | 2.25                     | 0.67              |
| 35:DA:1183:G:O2'   | 35:DA:1184:G:H5'   | 1.94                     | 0.67              |
| 35:DA:491:G:H2'    | 35:DA:492:A:H8     | 1.60                     | 0.67              |
| 37:DC:128:LEU:HD12 | 37:DC:131:ILE:HB   | 1.76                     | 0.67              |
| 39:DE:179:GLU:O    | 39:DE:180:ASN:HB2  | 1.94                     | 0.67              |
| 42:DH:76:VAL:O     | 42:DH:79:VAL:HG22  | 1.95                     | 0.67              |
| 46:DN:48:MET:CE    | 46:DN:48:MET:H     | 2.07                     | 0.67              |
| 48:DP:30:THR:CG2   | 48:DP:31:ALA:H     | 2.07                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:DP:38:GLN:HG3  | 48:DP:39:LYS:N     | 2.08                     | 0.67              |
| 48:DP:62:LEU:N    | 48:DP:62:LEU:HD23  | 2.09                     | 0.67              |
| 58:DZ:95:PRO:HA   | 58:DZ:129:SER:HA   | 1.77                     | 0.67              |
| 1:AA:942:G:H21    | 9:AI:124:GLN:NE2   | 1.92                     | 0.67              |
| 3:AC:206:GLU:HG2  | 3:AC:207:VAL:H     | 1.59                     | 0.67              |
| 9:AI:40:LEU:HD11  | 9:AI:70:LYS:HG2    | 1.75                     | 0.67              |
| 10:AJ:3:LYS:O     | 10:AJ:100:THR:HG23 | 1.95                     | 0.67              |
| 24:AY:404:VAL:N   | 24:AY:405:PRO:HD3  | 2.11                     | 0.67              |
| 24:AY:526:VAL:HB  | 24:AY:566:THR:HA   | 1.77                     | 0.67              |
| 26:B1:26:ARG:HG3  | 26:B1:27:GLU:H     | 1.60                     | 0.67              |
| 33:B8:50:LEU:CD1  | 33:B8:51:ALA:H     | 2.08                     | 0.67              |
| 35:BA:1541:G:H4'  | 35:BA:1542:A:C5'   | 2.25                     | 0.67              |
| 40:BF:192:LEU:C   | 40:BF:192:LEU:HD23 | 2.16                     | 0.67              |
| 41:BG:112:PRO:O   | 41:BG:113:ARG:CA   | 2.36                     | 0.67              |
| 51:BS:19:LYS:HB3  | 51:BS:20:ARG:NH2   | 2.10                     | 0.67              |
| 51:BS:58:LEU:HD12 | 51:BS:59:LYS:H     | 1.59                     | 0.67              |
| 54:BV:19:LYS:HE2  | 54:BV:20:LEU:H     | 1.61                     | 0.67              |
| 1:CA:1292:U:H2'   | 1:CA:1293:G:C8     | 2.30                     | 0.67              |
| 1:CA:1308:U:H5''  | 13:CM:98:VAL:HG23  | 1.75                     | 0.67              |
| 1:CA:294:U:H2'    | 1:CA:295:C:C6      | 2.30                     | 0.67              |
| 1:CA:980:C:C5     | 1:CA:981:U:C2      | 2.83                     | 0.67              |
| 9:CI:4:TYR:CD2    | 9:CI:88:TYR:HB2    | 2.29                     | 0.67              |
| 24:CY:21:ILE:HD13 | 24:CY:21:ILE:H     | 1.60                     | 0.67              |
| 24:CY:343:ASN:C   | 24:CY:343:ASN:HD22 | 1.99                     | 0.67              |
| 35:DA:1058:G:N2   | 35:DA:1081:U:H1'   | 2.10                     | 0.67              |
| 35:DA:1494:A:H2'  | 35:DA:1495:A:H5''  | 1.76                     | 0.67              |
| 35:DA:1644:C:O2   | 35:DA:1644:C:H2'   | 1.94                     | 0.67              |
| 35:DA:2241:A:H2'  | 35:DA:2242:G:C8    | 2.30                     | 0.67              |
| 35:DA:2408:U:H2'  | 35:DA:2409:G:H8    | 1.60                     | 0.67              |
| 44:DK:7:VAL:O     | 44:DK:7:VAL:HG13   | 1.94                     | 0.67              |
| 51:DS:98:VAL:HG12 | 51:DS:100:ALA:H    | 1.59                     | 0.67              |
| 51:DS:58:LEU:HD12 | 51:DS:59:LYS:H     | 1.60                     | 0.67              |
| 1:AA:1292:U:H2'   | 1:AA:1293:G:C8     | 2.30                     | 0.66              |
| 22:AV:17:C:H6     | 22:AV:17(A):U:H5   | 1.40                     | 0.66              |
| 24:AY:230:LYS:HE2 | 24:AY:241:GLU:OE1  | 1.95                     | 0.66              |
| 35:BA:1656:C:H2'  | 35:BA:1657:C:C6    | 2.29                     | 0.66              |
| 35:BA:1902:C:H4'  | 38:BD:244:ARG:HB2  | 1.77                     | 0.66              |
| 35:BA:389:G:H1    | 48:BP:71:VAL:HG12  | 1.60                     | 0.66              |
| 35:BA:936:C:H2'   | 35:BA:937:U:C6     | 2.30                     | 0.66              |
| 40:BF:89:VAL:HG12 | 40:BF:90:PHE:N     | 2.09                     | 0.66              |
| 44:BK:14:ALA:HA   | 44:BK:41:PHE:CE2   | 2.30                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:BO:35:VAL:HG11  | 47:BO:103:ALA:HB3  | 1.77                     | 0.66              |
| 53:BU:112:ARG:NH2  | 54:BV:46:VAL:HG11  | 2.10                     | 0.66              |
| 53:BU:113:ALA:C    | 53:BU:115:ALA:H    | 1.97                     | 0.66              |
| 53:BU:95:LEU:HD12  | 54:BV:11:GLN:HG3   | 1.76                     | 0.66              |
| 1:CA:1368:G:O2'    | 1:CA:1369:C:H5'    | 1.95                     | 0.66              |
| 1:CA:1190:G:OP1    | 3:CC:5:ILE:HD12    | 1.94                     | 0.66              |
| 6:CF:80:ARG:HH11   | 6:CF:88:VAL:HB     | 1.59                     | 0.66              |
| 10:CJ:42:THR:HG23  | 10:CJ:68:HIS:HA    | 1.77                     | 0.66              |
| 13:CM:97:PRO:CA    | 13:CM:110:ARG:HD3  | 2.25                     | 0.66              |
| 16:CP:33:ILE:O     | 16:CP:34:GLU:HB2   | 1.94                     | 0.66              |
| 16:CP:74:LEU:HD23  | 16:CP:79:VAL:HG21  | 1.74                     | 0.66              |
| 19:CS:20:LEU:HA    | 19:CS:23:ASN:HB2   | 1.75                     | 0.66              |
| 28:D3:6:VAL:HB     | 28:D3:54:VAL:HG11  | 1.77                     | 0.66              |
| 35:DA:1242:A:N1    | 48:DP:8:PRO:HG2    | 2.09                     | 0.66              |
| 35:DA:1682:G:H2'   | 35:DA:1683:C:H6    | 1.59                     | 0.66              |
| 35:DA:1567:A:H2'   | 38:DD:84:TYR:HE2   | 1.58                     | 0.66              |
| 39:DE:26:ILE:HG21  | 39:DE:196:VAL:HG21 | 1.77                     | 0.66              |
| 44:DK:77:LEU:HD23  | 44:DK:77:LEU:N     | 2.10                     | 0.66              |
| 51:DS:74:ALA:HB1   | 51:DS:103:GLU:CB   | 2.24                     | 0.66              |
| 51:DS:19:LYS:HB3   | 51:DS:20:ARG:NH2   | 2.10                     | 0.66              |
| 52:DT:115:ARG:HH11 | 52:DT:115:ARG:CB   | 2.04                     | 0.66              |
| 55:DW:64:MET:O     | 55:DW:65:LEU:HB3   | 1.94                     | 0.66              |
| 1:AA:491:G:H2'     | 1:AA:492:G:H8      | 1.59                     | 0.66              |
| 13:AM:10:PRO:HG2   | 13:AM:11:ARG:H     | 1.61                     | 0.66              |
| 14:AN:12:ARG:C     | 14:AN:14:PRO:HD3   | 2.16                     | 0.66              |
| 29:B4:14:ILE:N     | 29:B4:14:ILE:HD12  | 2.10                     | 0.66              |
| 35:BA:1115:G:H8    | 35:BA:1115:G:H5'   | 1.60                     | 0.66              |
| 35:BA:142:A:H5'    | 35:BA:142(A):C:OP2 | 1.95                     | 0.66              |
| 35:BA:1788:C:O2'   | 35:BA:1789:A:H5'   | 1.95                     | 0.66              |
| 35:BA:1846:G:H5'   | 35:BA:1846:G:C8    | 2.24                     | 0.66              |
| 35:BA:229:A:H3'    | 35:BA:230:U:H5'    | 1.77                     | 0.66              |
| 35:BA:2408:U:H2'   | 35:BA:2409:G:H8    | 1.59                     | 0.66              |
| 35:BA:2476:A:N1    | 35:BA:2477:C:C5    | 2.63                     | 0.66              |
| 35:BA:940:G:H3'    | 35:BA:941:A:H5''   | 1.77                     | 0.66              |
| 38:BD:166:GLN:HA   | 38:BD:166:GLN:HE21 | 1.61                     | 0.66              |
| 48:BP:122:PRO:HB3  | 48:BP:141:ALA:HB1  | 1.77                     | 0.66              |
| 52:BT:30:VAL:HG21  | 52:BT:84:GLN:H     | 1.61                     | 0.66              |
| 1:CA:1160:G:N3     | 1:CA:1160:G:H2'    | 2.10                     | 0.66              |
| 2:CB:27:LYS:HD3    | 2:CB:195:ASP:OD1   | 1.95                     | 0.66              |
| 24:CY:489:LYS:HD3  | 24:CY:598:ASP:OD1  | 1.93                     | 0.66              |
| 35:DA:657:U:H2'    | 35:DA:658:C:C6     | 2.31                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:DF:152:GLU:O    | 40:DF:154:VAL:HG23 | 1.94                     | 0.66              |
| 44:DK:109:LYS:O    | 44:DK:112:MET:HG2  | 1.94                     | 0.66              |
| 44:DK:23:VAL:HG13  | 44:DK:27:LEU:HD22  | 1.76                     | 0.66              |
| 51:DS:85:VAL:C     | 51:DS:106:ARG:HG2  | 2.16                     | 0.66              |
| 51:DS:19:LYS:HB3   | 51:DS:20:ARG:HH22  | 1.60                     | 0.66              |
| 52:DT:28:VAL:HG21  | 52:DT:46:GLU:CG    | 2.22                     | 0.66              |
| 52:DT:57:PHE:O     | 52:DT:59:THR:HG23  | 1.96                     | 0.66              |
| 53:DU:107:ALA:HA   | 53:DU:110:VAL:HG23 | 1.77                     | 0.66              |
| 1:AA:473:G:H2'     | 1:AA:474:G:H8      | 1.60                     | 0.66              |
| 2:AB:77:ALA:HB2    | 2:AB:211:ILE:HD13  | 1.76                     | 0.66              |
| 4:AD:30:LYS:C      | 4:AD:32:ALA:N      | 2.47                     | 0.66              |
| 13:AM:108:ARG:HH11 | 13:AM:108:ARG:HA   | 1.59                     | 0.66              |
| 24:AY:100:VAL:HG23 | 24:AY:329:ARG:HG2  | 1.76                     | 0.66              |
| 61:AY:702:FUA:H201 | 61:AY:702:FUA:O1   | 1.95                     | 0.66              |
| 24:AY:84:THR:N     | 24:AY:85:PRO:CD    | 2.55                     | 0.66              |
| 26:B1:73:LEU:HD23  | 26:B1:94:LEU:HD23  | 1.78                     | 0.66              |
| 35:BA:1028:A:N6    | 35:BA:1125:G:H2'   | 2.10                     | 0.66              |
| 35:BA:1917:U:C2'   | 35:BA:1918:A:H5'   | 2.25                     | 0.66              |
| 46:BN:58:ASP:OD2   | 46:BN:59:LYS:HG2   | 1.95                     | 0.66              |
| 48:BP:115:LEU:HD23 | 48:BP:115:LEU:N    | 2.10                     | 0.66              |
| 48:BP:7:ARG:CB     | 48:BP:8:PRO:HD3    | 2.23                     | 0.66              |
| 51:BS:85:VAL:C     | 51:BS:106:ARG:HG2  | 2.16                     | 0.66              |
| 1:CA:1238:A:N7     | 1:CA:1303:C:H1'    | 2.10                     | 0.66              |
| 3:CC:58:GLU:HB2    | 3:CC:65:ALA:HB2    | 1.78                     | 0.66              |
| 35:DA:1514:U:H2'   | 35:DA:1515:G:H8    | 1.61                     | 0.66              |
| 35:DA:1656:C:H2'   | 35:DA:1657:C:C6    | 2.31                     | 0.66              |
| 35:DA:2346:A:C2    | 35:DA:2383:G:C2    | 2.84                     | 0.66              |
| 35:DA:363(B):G:H2' | 35:DA:363(C):G:H8  | 1.59                     | 0.66              |
| 41:DG:45:GLU:O     | 41:DG:51:ARG:HB3   | 1.96                     | 0.66              |
| 48:DP:108:LYS:C    | 48:DP:110:TYR:H    | 1.98                     | 0.66              |
| 51:DS:104:GLY:C    | 51:DS:106:ARG:H    | 1.99                     | 0.66              |
| 2:AB:222:ILE:HB    | 2:AB:226:ARG:HH21  | 1.59                     | 0.66              |
| 2:AB:27:LYS:HD3    | 2:AB:195:ASP:OD1   | 1.94                     | 0.66              |
| 3:AC:137:ALA:HA    | 3:AC:140:ARG:NH2   | 2.09                     | 0.66              |
| 9:AI:5:TYR:CD2     | 9:AI:6:GLY:N       | 2.64                     | 0.66              |
| 11:AK:16:SER:O     | 11:AK:35:PRO:HG3   | 1.95                     | 0.66              |
| 20:AT:48:LYS:HB3   | 20:AT:51:GLU:HG2   | 1.78                     | 0.66              |
| 24:AY:119:GLU:O    | 24:AY:121:VAL:HG22 | 1.96                     | 0.66              |
| 26:B1:45:ASN:HD22  | 26:B1:46:LEU:N     | 1.92                     | 0.66              |
| 26:B1:64:ALA:HA    | 26:B1:67:ILE:HG13  | 1.76                     | 0.66              |
| 27:B2:13:ALA:HA    | 27:B2:16:LEU:CD1   | 2.26                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:B3:6:VAL:HB    | 28:B3:54:VAL:HG11 | 1.76                     | 0.66              |
| 35:BA:191:A:H2'   | 35:BA:192:C:H6    | 1.60                     | 0.66              |
| 35:BA:2713:A:H3'  | 35:BA:2714:G:C5'  | 2.25                     | 0.66              |
| 36:BB:26:A:H2'    | 36:BB:27:C:C6     | 2.30                     | 0.66              |
| 39:BE:199:ARG:HB3 | 39:BE:200:GLU:OE2 | 1.95                     | 0.66              |
| 40:BF:65:TRP:CZ3  | 40:BF:75:HIS:HD2  | 2.12                     | 0.66              |
| 41:BG:90:LEU:HD12 | 41:BG:91:ARG:H    | 1.59                     | 0.66              |
| 50:BR:10:LEU:HD22 | 50:BR:17:ARG:HD3  | 1.77                     | 0.66              |
| 57:BY:28:LYS:C    | 57:BY:38:ILE:HG22 | 2.16                     | 0.66              |
| 1:CA:1294:G:O2'   | 1:CA:1295:G:H5'   | 1.95                     | 0.66              |
| 1:CA:1323:G:H2'   | 1:CA:1324:A:H8    | 1.61                     | 0.66              |
| 6:CF:16:GLN:N     | 6:CF:16:GLN:CD    | 2.49                     | 0.66              |
| 24:CY:17:ILE:HD12 | 24:CY:17:ILE:N    | 2.08                     | 0.66              |
| 26:D1:80:LEU:HB3  | 26:D1:82:LEU:HD11 | 1.76                     | 0.66              |
| 31:D6:45:LYS:HD3  | 35:DA:2371:G:O3'  | 1.96                     | 0.66              |
| 35:DA:2425:A:H4'  | 35:DA:2426:A:H5'' | 1.75                     | 0.66              |
| 35:DA:2668:G:O2'  | 35:DA:2669:G:H5'  | 1.95                     | 0.66              |
| 38:DD:226:MET:HB3 | 38:DD:230:ASP:HB2 | 1.77                     | 0.66              |
| 44:DK:21:PRO:HG3  | 44:DK:25:PRO:HD3  | 1.77                     | 0.66              |
| 54:DV:19:LYS:HE2  | 54:DV:20:LEU:H    | 1.59                     | 0.66              |
| 1:AA:474:G:H2'    | 1:AA:475:G:H8     | 1.58                     | 0.66              |
| 1:AA:584:G:H2'    | 1:AA:585:G:C8     | 2.30                     | 0.66              |
| 1:AA:748:C:H6     | 1:AA:748:C:OP2    | 1.79                     | 0.66              |
| 9:AI:104:ARG:O    | 9:AI:105:ASP:HB3  | 1.94                     | 0.66              |
| 16:AP:33:ILE:O    | 16:AP:34:GLU:HB2  | 1.94                     | 0.66              |
| 29:B4:9:LEU:HD23  | 41:BG:65:GLY:HA3  | 1.76                     | 0.66              |
| 35:BA:1010:A:H1'  | 35:BA:1153:C:H1'  | 1.76                     | 0.66              |
| 35:BA:2631:G:N2   | 39:BE:61:ARG:HH12 | 1.93                     | 0.66              |
| 38:BD:91:ARG:NH1  | 38:BD:91:ARG:HG2  | 2.04                     | 0.66              |
| 42:BH:76:VAL:O    | 42:BH:79:VAL:HG22 | 1.95                     | 0.66              |
| 43:BJ:73:UNK:C    | 43:BJ:75:UNK:N    | 2.53                     | 0.66              |
| 44:BK:109:LYS:O   | 44:BK:112:MET:HG2 | 1.95                     | 0.66              |
| 1:CA:748:C:OP2    | 1:CA:748:C:H6     | 1.78                     | 0.66              |
| 7:CG:27:ILE:CD1   | 7:CG:40:ALA:HA    | 2.26                     | 0.66              |
| 24:CY:632:LEU:CG  | 24:CY:645:ALA:HA  | 2.26                     | 0.66              |
| 35:DA:2248:C:C2'  | 35:DA:2249:U:H5'  | 2.24                     | 0.66              |
| 42:DH:124:GLU:CB  | 42:DH:132:ARG:HG3 | 2.25                     | 0.66              |
| 49:DQ:55:VAL:CG1  | 49:DQ:56:ARG:N    | 2.59                     | 0.66              |
| 51:DS:40:ILE:HG22 | 51:DS:41:ASP:N    | 2.09                     | 0.66              |
| 53:DU:61:TRP:O    | 53:DU:65:ILE:HG13 | 1.95                     | 0.66              |
| 55:DW:5:ALA:O     | 55:DW:6:ILE:HB    | 1.93                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:DY:8:LYS:HB2    | 57:DY:28:LYS:HZ3   | 1.61                     | 0.66              |
| 58:DZ:77:ASP:HB2   | 58:DZ:82:ARG:HB3   | 1.78                     | 0.66              |
| 1:AA:1160:G:N3     | 1:AA:1160:G:H2'    | 2.09                     | 0.66              |
| 1:AA:294:U:H2'     | 1:AA:295:C:C6      | 2.29                     | 0.66              |
| 9:AI:53:VAL:C      | 9:AI:55:ALA:H      | 1.99                     | 0.66              |
| 10:AJ:42:THR:HG23  | 10:AJ:68:HIS:HA    | 1.76                     | 0.66              |
| 10:AJ:32:ALA:HB2   | 10:AJ:76:ASN:ND2   | 2.10                     | 0.66              |
| 17:AQ:47:PRO:HG2   | 17:AQ:48:GLU:OE2   | 1.96                     | 0.66              |
| 31:B6:10:LEU:HD22  | 31:B6:10:LEU:H     | 1.59                     | 0.66              |
| 35:BA:1217:C:OP2   | 53:BU:15:LYS:NZ    | 2.23                     | 0.66              |
| 35:BA:1223:G:C3'   | 35:BA:1224:C:H5''  | 2.24                     | 0.66              |
| 35:BA:1917:U:O2'   | 35:BA:1918:A:H5'   | 1.95                     | 0.66              |
| 35:BA:2162:G:H2'   | 35:BA:2163:C:C6    | 2.31                     | 0.66              |
| 35:BA:2196:C:O2'   | 35:BA:2197:U:H5'   | 1.96                     | 0.66              |
| 35:BA:2591:C:OP2   | 38:BD:239:ARG:HB3  | 1.96                     | 0.66              |
| 37:BC:48:LEU:HD12  | 37:BC:48:LEU:N     | 2.11                     | 0.66              |
| 46:BN:21:LYS:HB3   | 46:BN:26:LEU:HD23  | 1.78                     | 0.66              |
| 46:BN:67:LEU:HB3   | 46:BN:88:GLU:CG    | 2.26                     | 0.66              |
| 48:BP:114:ILE:HD12 | 48:BP:115:LEU:N    | 2.11                     | 0.66              |
| 52:BT:85:LYS:HB3   | 52:BT:85:LYS:HZ2   | 1.59                     | 0.66              |
| 57:BY:51:VAL:C     | 57:BY:53:PRO:HD2   | 2.16                     | 0.66              |
| 3:CC:58:GLU:N      | 3:CC:65:ALA:HB3    | 2.06                     | 0.66              |
| 5:CE:36:ASP:O      | 5:CE:37:ARG:HB2    | 1.96                     | 0.66              |
| 1:CA:973:G:H1'     | 10:CJ:55:LYS:HZ1   | 1.61                     | 0.66              |
| 29:D4:1:MET:HG2    | 41:DG:98:ARG:CZ    | 2.25                     | 0.66              |
| 35:DA:1113:U:H2'   | 35:DA:1114:G:C8    | 2.30                     | 0.66              |
| 35:DA:1268:A:H2'   | 35:DA:1269:A:O4'   | 1.96                     | 0.66              |
| 35:DA:145:G:H2'    | 35:DA:146:G:H8     | 1.61                     | 0.66              |
| 35:DA:2346:A:H1'   | 35:DA:2383:G:C8    | 2.30                     | 0.66              |
| 35:DA:2893:G:H5'   | 35:DA:2894:G:H5'   | 1.78                     | 0.66              |
| 35:DA:580:C:H2'    | 35:DA:581:C:C6     | 2.31                     | 0.66              |
| 38:DD:117:VAL:HG23 | 38:DD:129:ASN:HA   | 1.75                     | 0.66              |
| 38:DD:158:ALA:O    | 38:DD:196:VAL:HG11 | 1.96                     | 0.66              |
| 39:DE:11:MET:CB    | 39:DE:24:THR:HA    | 2.25                     | 0.66              |
| 48:DP:114:ILE:HD12 | 48:DP:115:LEU:N    | 2.09                     | 0.66              |
| 35:DA:807:U:OP2    | 48:DP:39:LYS:HG3   | 1.94                     | 0.66              |
| 51:DS:15:ARG:HB3   | 51:DS:18:ILE:CD1   | 2.24                     | 0.66              |
| 53:DU:111:GLU:O    | 53:DU:115:ALA:HB2  | 1.95                     | 0.66              |
| 58:DZ:143:GLY:O    | 58:DZ:144:LEU:HD13 | 1.96                     | 0.66              |
| 1:AA:1261:A:H2'    | 1:AA:1262:C:H5'    | 1.76                     | 0.66              |
| 1:AA:1324:A:H2'    | 1:AA:1325:C:C6     | 2.31                     | 0.66              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:191:G:C4      | 20:AT:105:SER:HB3  | 2.30                     | 0.66              |
| 4:AD:24:GLU:O      | 4:AD:27:TYR:HB2    | 1.96                     | 0.66              |
| 11:AK:48:ILE:HD13  | 11:AK:48:ILE:N     | 2.10                     | 0.66              |
| 16:AP:8:ARG:HB3    | 16:AP:28:ARG:HH12  | 1.60                     | 0.66              |
| 31:B6:27:LYS:HD2   | 31:B6:30:THR:HB    | 1.78                     | 0.66              |
| 32:B7:46:VAL:HG12  | 32:B7:47:ARG:N     | 2.11                     | 0.66              |
| 35:BA:2241:A:H2'   | 35:BA:2242:G:C8    | 2.30                     | 0.66              |
| 38:BD:153:ALA:C    | 38:BD:154:LYS:HG3  | 2.16                     | 0.66              |
| 41:BG:28:VAL:O     | 41:BG:31:VAL:HG12  | 1.95                     | 0.66              |
| 48:BP:41:ARG:CA    | 48:BP:41:ARG:HH21  | 2.05                     | 0.66              |
| 58:BZ:18:LEU:O     | 58:BZ:21:ALA:HB3   | 1.96                     | 0.66              |
| 58:BZ:4:ARG:NH1    | 58:BZ:66:SER:HB2   | 2.10                     | 0.66              |
| 1:CA:1347:G:H3'    | 9:CI:108:VAL:O     | 1.95                     | 0.66              |
| 1:CA:1412:C:H2'    | 1:CA:1413:A:C8     | 2.29                     | 0.66              |
| 1:CA:20:U:H2'      | 1:CA:21:G:O4'      | 1.95                     | 0.66              |
| 11:CK:16:SER:O     | 11:CK:35:PRO:HG3   | 1.95                     | 0.66              |
| 19:CS:6:LYS:H      | 19:CS:6:LYS:CE     | 2.09                     | 0.66              |
| 26:D1:8:SER:HB3    | 26:D1:66:HIS:CE1   | 2.31                     | 0.66              |
| 28:D3:28:LEU:N     | 28:D3:28:LEU:HD23  | 2.10                     | 0.66              |
| 31:D6:19:ARG:O     | 31:D6:20:ASN:O     | 2.14                     | 0.66              |
| 33:D8:6:THR:CG2    | 33:D8:63:PRO:HD3   | 2.25                     | 0.66              |
| 35:DA:2206:G:N2    | 35:DA:2207:G:H5'   | 2.11                     | 0.66              |
| 35:DA:784:A:H5''   | 38:DD:227:ASN:ND2  | 2.11                     | 0.66              |
| 35:DA:903:C:H2'    | 35:DA:904:C:C5'    | 2.18                     | 0.66              |
| 36:DB:26:A:H2'     | 36:DB:27:C:C6      | 2.31                     | 0.66              |
| 41:DG:123:ASN:C    | 41:DG:125:PHE:H    | 1.99                     | 0.66              |
| 47:DO:64:ARG:O     | 47:DO:82:ASN:HA    | 1.96                     | 0.66              |
| 54:DV:19:LYS:CE    | 54:DV:20:LEU:H     | 2.09                     | 0.66              |
| 1:AA:1238:A:N7     | 1:AA:1303:C:H1'    | 2.11                     | 0.66              |
| 1:AA:715:A:H2'     | 1:AA:716:A:C8      | 2.30                     | 0.66              |
| 24:AY:466:LEU:HA   | 24:AY:470:PHE:HD2  | 1.58                     | 0.66              |
| 32:B7:28:ARG:HG3   | 32:B7:28:ARG:HH11  | 1.60                     | 0.66              |
| 35:BA:2206:G:N2    | 35:BA:2207:G:H5'   | 2.11                     | 0.66              |
| 40:BF:125:LEU:H    | 40:BF:125:LEU:HD23 | 1.60                     | 0.66              |
| 44:BK:57:ILE:N     | 44:BK:57:ILE:HD12  | 2.11                     | 0.66              |
| 1:CA:1234:C:O2'    | 1:CA:1235:U:H5'    | 1.96                     | 0.66              |
| 35:DA:27:G:HO2'    | 35:DA:28:A:H8      | 1.41                     | 0.66              |
| 37:DC:134:PRO:C    | 37:DC:135:ARG:HD2  | 2.15                     | 0.66              |
| 38:DD:35:LYS:HD2   | 38:DD:36:PRO:CA    | 2.25                     | 0.66              |
| 40:DF:125:LEU:HD23 | 40:DF:125:LEU:H    | 1.61                     | 0.66              |
| 51:DS:67:ARG:HB3   | 51:DS:71:ARG:HH22  | 1.61                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:DS:95:HIS:CG    | 51:DS:96:GLY:N     | 2.62                     | 0.66              |
| 57:DY:76:CYS:HB3   | 57:DY:96:ILE:CD1   | 2.22                     | 0.66              |
| 1:AA:1321:C:H5''   | 1:AA:1322:C:C5'    | 2.26                     | 0.66              |
| 1:AA:1346:A:N1     | 1:AA:1374:A:H5''   | 2.11                     | 0.66              |
| 1:AA:630:G:C2'     | 1:AA:631:G:H5''    | 2.26                     | 0.66              |
| 3:AC:11:ARG:O      | 3:AC:13:GLY:N      | 2.29                     | 0.66              |
| 3:AC:58:GLU:N      | 3:AC:65:ALA:HB3    | 2.07                     | 0.66              |
| 5:AE:91:LEU:HD13   | 5:AE:120:THR:CG2   | 2.25                     | 0.66              |
| 6:AF:80:ARG:HH11   | 6:AF:88:VAL:HB     | 1.60                     | 0.66              |
| 10:AJ:49:VAL:CG2   | 14:AN:41:ARG:HB2   | 2.24                     | 0.66              |
| 12:AL:18:VAL:O     | 12:AL:19:ARG:HB3   | 1.96                     | 0.66              |
| 24:AY:485:GLU:HG3  | 24:AY:553:GLY:HA3  | 1.77                     | 0.66              |
| 24:AY:517:LEU:HB3  | 24:AY:521:SER:CB   | 2.26                     | 0.66              |
| 35:BA:1080:C:O2'   | 35:BA:1081:U:H5'   | 1.96                     | 0.66              |
| 35:BA:2069:G:O2'   | 35:BA:2070:G:H5'   | 1.96                     | 0.66              |
| 35:BA:2241:A:H2'   | 35:BA:2242:G:H8    | 1.60                     | 0.66              |
| 39:BE:26:ILE:HG21  | 39:BE:196:VAL:HG21 | 1.77                     | 0.66              |
| 40:BF:132:VAL:HG22 | 40:BF:133:ASN:N    | 2.11                     | 0.66              |
| 40:BF:4:VAL:HG13   | 40:BF:19:GLU:OE2   | 1.95                     | 0.66              |
| 41:BG:56:ALA:HB1   | 41:BG:153:ARG:NE   | 2.11                     | 0.66              |
| 42:BH:154:PRO:O    | 42:BH:156:ALA:N    | 2.27                     | 0.66              |
| 44:BK:6:ALA:CB     | 44:BK:59:ILE:HG22  | 2.21                     | 0.66              |
| 44:BK:93:ARG:HB2   | 58:BZ:112:ARG:NE   | 2.09                     | 0.66              |
| 52:BT:106:SER:HA   | 52:BT:110:ILE:HG12 | 1.78                     | 0.66              |
| 58:BZ:82:ARG:O     | 58:BZ:83:PRO:C     | 2.32                     | 0.66              |
| 1:CA:1261:A:H2'    | 1:CA:1262:C:H5'    | 1.77                     | 0.66              |
| 1:CA:41:G:H2'      | 1:CA:42:G:H8       | 1.59                     | 0.66              |
| 2:CB:189:ASP:OD1   | 2:CB:205:ASP:HB3   | 1.95                     | 0.66              |
| 2:CB:54:THR:O      | 2:CB:58:ILE:HG13   | 1.95                     | 0.66              |
| 3:CC:70:VAL:CG1    | 3:CC:72:LYS:H      | 2.03                     | 0.66              |
| 10:CJ:3:LYS:O      | 10:CJ:100:THR:HG23 | 1.96                     | 0.66              |
| 22:CW:52:C:H3'     | 22:CW:53:G:H5''    | 1.77                     | 0.66              |
| 22:CW:37:U:H3      | 23:CX:13:A:H61     | 1.44                     | 0.66              |
| 24:CY:115:GLU:OE1  | 24:CY:152:THR:HG21 | 1.96                     | 0.66              |
| 24:CY:530:VAL:HG12 | 24:CY:533:VAL:HG23 | 1.78                     | 0.66              |
| 24:CY:26:THR:HA    | 24:CY:83:ASP:OD1   | 1.95                     | 0.66              |
| 24:CY:99:ARG:HE    | 24:CY:128:TYR:HB2  | 1.61                     | 0.66              |
| 35:DA:1278:A:H5''  | 50:DR:36:THR:HG22  | 1.77                     | 0.66              |
| 35:DA:191:A:H2'    | 35:DA:192:C:H6     | 1.60                     | 0.66              |
| 30:D5:19:ARG:HA    | 35:DA:2046:G:H5'   | 1.78                     | 0.66              |
| 35:DA:279:C:C2'    | 35:DA:280:C:H5''   | 2.25                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:DD:35:LYS:HG2   | 38:DD:63:ARG:CA    | 2.24                     | 0.66              |
| 41:DG:139:LEU:HA   | 41:DG:144:ILE:HG21 | 1.78                     | 0.66              |
| 41:DG:62:LEU:HD12  | 41:DG:62:LEU:N     | 2.04                     | 0.66              |
| 44:DK:57:ILE:N     | 44:DK:57:ILE:HD12  | 2.10                     | 0.66              |
| 44:DK:56:GLU:O     | 44:DK:67:PHE:HA    | 1.96                     | 0.66              |
| 51:DS:49:VAL:HG12  | 51:DS:50:SER:N     | 2.11                     | 0.66              |
| 56:DX:35:THR:HB    | 56:DX:38:GLU:HB2   | 1.77                     | 0.66              |
| 57:DY:88:LYS:O     | 57:DY:90:LEU:HD23  | 1.95                     | 0.66              |
| 1:AA:188:C:H2'     | 1:AA:189:G:H8      | 1.61                     | 0.66              |
| 8:AH:10:LEU:CD2    | 8:AH:83:ILE:HD11   | 2.24                     | 0.66              |
| 24:AY:12:LEU:HB3   | 24:AY:283:PRO:HG2  | 1.78                     | 0.66              |
| 24:AY:17:ILE:O     | 24:AY:85:PRO:HG2   | 1.96                     | 0.66              |
| 27:B2:50:ILE:C     | 27:B2:52:ASP:H     | 1.96                     | 0.66              |
| 35:BA:1081:U:H5''  | 44:BK:122:ALA:HB1  | 1.77                     | 0.66              |
| 35:BA:1494:A:H2'   | 35:BA:1495:A:H5''  | 1.78                     | 0.66              |
| 25:B0:16:SER:OG    | 35:BA:2261:C:H3'   | 1.96                     | 0.66              |
| 35:BA:295:G:H2'    | 35:BA:296:C:H6     | 1.61                     | 0.66              |
| 38:BD:24:ILE:HD13  | 38:BD:25:THR:N     | 2.10                     | 0.66              |
| 42:BH:124:GLU:HB2  | 42:BH:132:ARG:HG3  | 1.78                     | 0.66              |
| 44:BK:23:VAL:HG13  | 44:BK:27:LEU:HD22  | 1.77                     | 0.66              |
| 47:BO:104:ARG:HH21 | 52:BT:33:LYS:HE3   | 1.61                     | 0.66              |
| 48:BP:13:ASN:O     | 48:BP:14:LYS:HB2   | 1.96                     | 0.66              |
| 50:BR:30:THR:OG1   | 50:BR:75:LEU:HD21  | 1.95                     | 0.66              |
| 57:BY:74:PRO:O     | 57:BY:80:GLY:HA2   | 1.96                     | 0.66              |
| 58:BZ:99:TYR:HE2   | 58:BZ:125:LEU:HD13 | 1.61                     | 0.66              |
| 1:CA:1038:C:H2'    | 1:CA:1039:C:C5     | 2.30                     | 0.66              |
| 1:CA:584:G:H2'     | 1:CA:585:G:H8      | 1.59                     | 0.66              |
| 3:CC:58:GLU:H      | 3:CC:65:ALA:CB     | 2.06                     | 0.66              |
| 26:D1:46:LEU:CD2   | 26:D1:46:LEU:H     | 2.07                     | 0.66              |
| 26:D1:86:SER:HB2   | 26:D1:90:ILE:HG12  | 1.78                     | 0.66              |
| 35:DA:1052:C:H2'   | 35:DA:1053:C:C6    | 2.31                     | 0.66              |
| 35:DA:1115:G:H8    | 35:DA:1115:G:H5'   | 1.61                     | 0.66              |
| 35:DA:1028:A:N6    | 35:DA:1125:G:H2'   | 2.11                     | 0.66              |
| 35:DA:139:G:C6     | 35:DA:140:G:H2'    | 2.30                     | 0.66              |
| 35:DA:1516:C:H2'   | 35:DA:1517:G:H5'   | 1.78                     | 0.66              |
| 35:DA:1865:G:H2'   | 35:DA:1866:C:H5''  | 1.76                     | 0.66              |
| 35:DA:229:A:H3'    | 35:DA:230:U:H5'    | 1.77                     | 0.66              |
| 35:DA:2631:G:N2    | 39:DE:61:ARG:NH1   | 2.44                     | 0.66              |
| 35:DA:545:C:H3'    | 35:DA:547:A:H5''   | 1.78                     | 0.66              |
| 35:DA:559:G:H22    | 53:DU:49:HIS:CD2   | 2.14                     | 0.66              |
| 35:DA:606:U:O2     | 35:DA:606:U:H2'    | 1.96                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:814:C:H2'    | 35:DA:815:C:C6     | 2.30                     | 0.66              |
| 38:DD:43:ARG:HB3   | 38:DD:54:ARG:HB2   | 1.78                     | 0.66              |
| 38:DD:61:LEU:O     | 38:DD:63:ARG:NH1   | 2.29                     | 0.66              |
| 39:DE:11:MET:HB3   | 39:DE:24:THR:HA    | 1.78                     | 0.66              |
| 42:DH:137:ASP:HB3  | 42:DH:140:LYS:HB2  | 1.77                     | 0.66              |
| 42:DH:175:LYS:O    | 42:DH:176:ALA:HB3  | 1.97                     | 0.66              |
| 42:DH:37:VAL:HG12  | 42:DH:38:SER:N     | 2.10                     | 0.66              |
| 54:DV:39:LEU:O     | 54:DV:40:LEU:HB2   | 1.95                     | 0.66              |
| 57:DY:62:GLU:CG    | 57:DY:63:LYS:H     | 2.09                     | 0.66              |
| 58:DZ:12:GLY:HA2   | 58:DZ:36:LYS:HZ1   | 1.60                     | 0.66              |
| 4:AD:36:ARG:CB     | 4:AD:36:ARG:HH11   | 2.09                     | 0.65              |
| 24:AY:9:LEU:C      | 24:AY:9:LEU:HD23   | 2.17                     | 0.65              |
| 25:B0:40:GLN:HE22  | 25:B0:43:THR:HA    | 1.60                     | 0.65              |
| 31:B6:17:LYS:HB2   | 31:B6:44:ARG:HH12  | 1.60                     | 0.65              |
| 35:BA:1814:G:C3'   | 35:BA:1815:A:H5''  | 2.25                     | 0.65              |
| 35:BA:2186:G:H2'   | 35:BA:2187:G:H5''  | 1.78                     | 0.65              |
| 35:BA:271(J):C:H2' | 35:BA:271(J):C:O2  | 1.94                     | 0.65              |
| 35:BA:643:A:O2'    | 35:BA:644:A:H5'    | 1.96                     | 0.65              |
| 35:BA:759:G:H2'    | 35:BA:760:G:H8     | 1.61                     | 0.65              |
| 35:BA:803:U:O2'    | 35:BA:804:A:H5'    | 1.96                     | 0.65              |
| 35:BA:848:G:H5'    | 35:BA:849:A:OP2    | 1.97                     | 0.65              |
| 37:BC:134:PRO:C    | 37:BC:135:ARG:HD2  | 2.16                     | 0.65              |
| 39:BE:101:ARG:NH1  | 39:BE:169:ASN:HD22 | 1.94                     | 0.65              |
| 41:BG:31:VAL:CG2   | 41:BG:32:PRO:HD2   | 2.26                     | 0.65              |
| 46:BN:96:GLU:H     | 46:BN:96:GLU:CD    | 2.00                     | 0.65              |
| 49:BQ:55:VAL:CG1   | 49:BQ:56:ARG:N     | 2.59                     | 0.65              |
| 54:BV:19:LYS:CE    | 54:BV:20:LEU:H     | 2.09                     | 0.65              |
| 1:CA:1068:G:OP2    | 1:CA:1094:G:H5'    | 1.96                     | 0.65              |
| 1:CA:1250:A:H4'    | 9:CI:68:GLY:N      | 2.11                     | 0.65              |
| 1:CA:630:G:C2'     | 1:CA:631:G:H5''    | 2.26                     | 0.65              |
| 1:CA:943:U:H2'     | 1:CA:944:G:H5'     | 1.79                     | 0.65              |
| 4:CD:9:CYS:HA      | 4:CD:12:CYS:HB2    | 1.78                     | 0.65              |
| 10:CJ:33:GLN:O     | 10:CJ:75:ILE:HG12  | 1.95                     | 0.65              |
| 1:CA:625:G:H4'     | 16:CP:16:HIS:CD2   | 2.31                     | 0.65              |
| 24:CY:388:THR:HG21 | 24:CY:399:LEU:CD1  | 2.25                     | 0.65              |
| 31:D6:17:LYS:HB2   | 31:D6:44:ARG:HH12  | 1.61                     | 0.65              |
| 35:DA:2852:G:H2'   | 35:DA:2853:C:H6    | 1.60                     | 0.65              |
| 37:DC:4:HIS:ND1    | 37:DC:8:TYR:HE2    | 1.94                     | 0.65              |
| 41:DG:48:GLU:OE1   | 41:DG:81:LYS:HE3   | 1.96                     | 0.65              |
| 44:DK:19:PRO:CB    | 44:DK:34:ILE:HD12  | 2.23                     | 0.65              |
| 47:DO:104:ARG:HH21 | 52:DT:33:LYS:HE3   | 1.61                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:DO:35:VAL:HG11  | 47:DO:103:ALA:HB3  | 1.78                     | 0.65              |
| 48:DP:122:PRO:HB3  | 48:DP:141:ALA:HB1  | 1.78                     | 0.65              |
| 49:DQ:75:THR:HG22  | 49:DQ:76:LYS:N     | 2.11                     | 0.65              |
| 49:DQ:76:LYS:HB3   | 49:DQ:91:GLU:HG3   | 1.78                     | 0.65              |
| 51:DS:30:ARG:HD3   | 51:DS:97:ARG:HG2   | 1.78                     | 0.65              |
| 57:DY:81:LYS:HD3   | 57:DY:97:ARG:O     | 1.95                     | 0.65              |
| 58:DZ:137:ILE:CG2  | 58:DZ:155:LEU:HD12 | 2.26                     | 0.65              |
| 1:AA:490:G:H2'     | 1:AA:491:G:H8      | 1.60                     | 0.65              |
| 3:AC:136:GLN:HG3   | 3:AC:139:GLN:HB3   | 1.78                     | 0.65              |
| 4:AD:36:ARG:HB3    | 4:AD:36:ARG:HH11   | 1.61                     | 0.65              |
| 6:AF:19:LEU:HD23   | 6:AF:19:LEU:O      | 1.96                     | 0.65              |
| 24:AY:388:THR:HG21 | 24:AY:399:LEU:H    | 1.61                     | 0.65              |
| 31:B6:38:LYS:HD3   | 35:BA:2344:U:OP1   | 1.96                     | 0.65              |
| 35:BA:2552:U:C2    | 35:BA:2554:U:H5'   | 2.31                     | 0.65              |
| 35:BA:272(B):G:H2' | 35:BA:272(C):G:H8  | 1.61                     | 0.65              |
| 35:BA:545:C:H3'    | 35:BA:547:A:H5''   | 1.79                     | 0.65              |
| 40:BF:160:ASN:HD21 | 40:BF:162:LEU:HB2  | 1.60                     | 0.65              |
| 55:BW:5:ALA:O      | 55:BW:6:ILE:HB     | 1.95                     | 0.65              |
| 1:CA:1231:G:O2'    | 1:CA:1232:U:H5'    | 1.96                     | 0.65              |
| 1:CA:1321:C:H5''   | 1:CA:1322:C:C5'    | 2.26                     | 0.65              |
| 1:CA:1411:C:H2'    | 1:CA:1412:C:C6     | 2.31                     | 0.65              |
| 1:CA:865:A:H5'     | 1:CA:1078:U:O4     | 1.96                     | 0.65              |
| 14:CN:12:ARG:O     | 14:CN:14:PRO:HD3   | 1.96                     | 0.65              |
| 16:CP:28:ARG:HG2   | 16:CP:29:ASP:OD2   | 1.96                     | 0.65              |
| 31:D6:10:LEU:H     | 31:D6:10:LEU:HD23  | 1.61                     | 0.65              |
| 35:DA:284:U:H2'    | 35:DA:285:C:H6     | 1.61                     | 0.65              |
| 35:DA:1012:U:O4    | 46:DN:28:THR:HG21  | 1.96                     | 0.65              |
| 46:DN:43:THR:O     | 46:DN:46:VAL:HG12  | 1.94                     | 0.65              |
| 50:DR:18:LEU:HD21  | 50:DR:22:ARG:NE    | 2.10                     | 0.65              |
| 55:DW:68:ARG:HA    | 55:DW:110:LYS:HG2  | 1.77                     | 0.65              |
| 1:AA:1248:A:C2'    | 1:AA:1249:C:H5'    | 2.27                     | 0.65              |
| 1:AA:66:G:H4'      | 1:AA:173:U:C5      | 2.32                     | 0.65              |
| 2:AB:54:THR:O      | 2:AB:58:ILE:HG13   | 1.96                     | 0.65              |
| 5:AE:152:ARG:HB3   | 8:AH:43:GLY:HA3    | 1.78                     | 0.65              |
| 24:AY:400:GLU:O    | 24:AY:402:ILE:HD12 | 1.96                     | 0.65              |
| 24:AY:424:LEU:O    | 24:AY:427:ALA:HB3  | 1.95                     | 0.65              |
| 35:BA:2537:U:H2'   | 35:BA:2538:C:C6    | 2.31                     | 0.65              |
| 35:BA:2893:G:H5'   | 35:BA:2894:G:H5'   | 1.78                     | 0.65              |
| 35:BA:301:G:H1'    | 35:BA:302:C:C6     | 2.30                     | 0.65              |
| 35:BA:364:C:C2'    | 35:BA:365:C:H5''   | 2.25                     | 0.65              |
| 35:BA:657:U:H2'    | 35:BA:658:C:C6     | 2.32                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:BA:796:C:H2'   | 35:BA:797:C:C6     | 2.31                     | 0.65              |
| 41:BG:34:LEU:HA   | 41:BG:161:THR:HA   | 1.78                     | 0.65              |
| 42:BH:124:GLU:CB  | 42:BH:132:ARG:HG3  | 2.26                     | 0.65              |
| 44:BK:58:THR:O    | 44:BK:66:THR:HG22  | 1.96                     | 0.65              |
| 47:BO:107:ARG:O   | 47:BO:112:MET:HE1  | 1.97                     | 0.65              |
| 51:BS:104:GLY:C   | 51:BS:106:ARG:H    | 2.00                     | 0.65              |
| 53:BU:92:ARG:HD3  | 53:BU:94:ASN:HB3   | 1.78                     | 0.65              |
| 58:BZ:130:PRO:O   | 58:BZ:133:ILE:HD11 | 1.96                     | 0.65              |
| 58:BZ:24:LEU:HD12 | 58:BZ:41:LEU:CD2   | 2.27                     | 0.65              |
| 1:CA:191:G:C4     | 20:CT:105:SER:HB3  | 2.31                     | 0.65              |
| 1:CA:490:G:H2'    | 1:CA:491:G:H8      | 1.61                     | 0.65              |
| 1:CA:664:G:H22    | 1:CA:741:G:H1      | 1.44                     | 0.65              |
| 1:CA:697:U:C2'    | 1:CA:698:G:H5'     | 2.25                     | 0.65              |
| 4:CD:121:VAL:O    | 4:CD:134:ASP:HA    | 1.96                     | 0.65              |
| 4:CD:152:SER:O    | 4:CD:154:ASN:N     | 2.29                     | 0.65              |
| 24:CY:225:GLU:O   | 24:CY:228:MET:HB3  | 1.96                     | 0.65              |
| 26:D1:29:GLY:HA3  | 35:DA:2396:G:O2'   | 1.95                     | 0.65              |
| 35:DA:1080:C:O2'  | 35:DA:1081:U:H5'   | 1.97                     | 0.65              |
| 35:DA:2039:C:H2'  | 35:DA:2040:C:H6    | 1.60                     | 0.65              |
| 36:DB:15:A:H3'    | 36:DB:16:G:C5'     | 2.25                     | 0.65              |
| 52:DT:30:VAL:HG21 | 52:DT:84:GLN:H     | 1.62                     | 0.65              |
| 53:DU:92:ARG:HD3  | 53:DU:94:ASN:HB3   | 1.77                     | 0.65              |
| 1:AA:1305:G:N2    | 1:AA:1331:G:O2'    | 2.28                     | 0.65              |
| 13:AM:4:ILE:HG22  | 13:AM:5:ALA:N      | 2.11                     | 0.65              |
| 16:AP:60:LEU:HA   | 16:AP:64:ALA:HB3   | 1.78                     | 0.65              |
| 35:BA:2347:C:H2'  | 35:BA:2348:U:C6    | 2.31                     | 0.65              |
| 35:BA:803:U:C2'   | 35:BA:804:A:H5'    | 2.27                     | 0.65              |
| 35:BA:637:A:H2'   | 48:BP:117:GLU:OE2  | 1.95                     | 0.65              |
| 48:BP:23:PRO:HB2  | 48:BP:33:ARG:CD    | 2.26                     | 0.65              |
| 53:BU:61:TRP:O    | 53:BU:65:ILE:HG13  | 1.96                     | 0.65              |
| 56:BX:35:THR:HB   | 56:BX:38:GLU:HB2   | 1.79                     | 0.65              |
| 58:BZ:24:LEU:HD12 | 58:BZ:41:LEU:HD21  | 1.78                     | 0.65              |
| 7:CG:80:VAL:HG23  | 7:CG:81:GLY:N      | 2.12                     | 0.65              |
| 23:CX:16:A:H2'    | 23:CX:17:U:C6      | 2.31                     | 0.65              |
| 24:CY:448:GLN:OE1 | 24:CY:480:GLN:HG2  | 1.97                     | 0.65              |
| 24:CY:84:THR:HG22 | 24:CY:84:THR:O     | 1.96                     | 0.65              |
| 35:DA:1386:C:H2'  | 35:DA:1387:C:H6    | 1.62                     | 0.65              |
| 35:DA:1812:A:H2'  | 35:DA:1813:G:H8    | 1.62                     | 0.65              |
| 35:DA:2498:C:O2'  | 35:DA:2499:C:H5'   | 1.95                     | 0.65              |
| 35:DA:2750:A:H2'  | 35:DA:2752:C:H41   | 1.61                     | 0.65              |
| 43:DJ:21:UNK:CB   | 43:DJ:88:UNK:HA    | 2.26                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:DS:97:ARG:HH21  | 51:DS:98:VAL:HA    | 1.62                     | 0.65              |
| 35:DA:143(A):C:H4' | 56:DX:38:GLU:OE1   | 1.96                     | 0.65              |
| 58:DZ:101:PRO:O    | 58:DZ:102:LEU:HD23 | 1.96                     | 0.65              |
| 2:AB:168:THR:CG2   | 2:AB:192:SER:HB3   | 2.20                     | 0.65              |
| 14:AN:29:ARG:HG3   | 14:AN:29:ARG:HH11  | 1.62                     | 0.65              |
| 23:AX:11:U:H2'     | 23:AX:11:U:O2      | 1.97                     | 0.65              |
| 24:AY:416:LYS:HD2  | 24:AY:417:THR:H    | 1.60                     | 0.65              |
| 31:B6:11:LEU:HD23  | 31:B6:51:GLU:HG3   | 1.77                     | 0.65              |
| 36:BB:30:C:OP2     | 51:BS:32:LEU:HD11  | 1.97                     | 0.65              |
| 39:BE:11:MET:CB    | 39:BE:24:THR:HA    | 2.27                     | 0.65              |
| 40:BF:4:VAL:HG22   | 40:BF:19:GLU:OE1   | 1.96                     | 0.65              |
| 41:BG:90:LEU:HD12  | 41:BG:91:ARG:N     | 2.10                     | 0.65              |
| 43:BJ:26:UNK:HA    | 43:BJ:84:UNK:HA    | 1.78                     | 0.65              |
| 44:BK:21:PRO:HG3   | 44:BK:25:PRO:HD3   | 1.78                     | 0.65              |
| 48:BP:108:LYS:C    | 48:BP:110:TYR:H    | 1.98                     | 0.65              |
| 48:BP:95:VAL:HG23  | 48:BP:125:VAL:HG23 | 1.77                     | 0.65              |
| 36:BB:48:A:H4'     | 51:BS:95:HIS:CD2   | 2.30                     | 0.65              |
| 52:BT:80:SER:CB    | 52:BT:81:PRO:HD3   | 2.25                     | 0.65              |
| 1:CA:1220:G:H2'    | 1:CA:1221:G:H8     | 1.62                     | 0.65              |
| 2:CB:77:ALA:HB2    | 2:CB:211:ILE:HD13  | 1.77                     | 0.65              |
| 24:CY:165:GLN:C    | 24:CY:166:LEU:HD12 | 2.17                     | 0.65              |
| 24:CY:25:LYS:HE2   | 24:CY:86:GLY:N     | 2.11                     | 0.65              |
| 24:CY:12:LEU:O     | 24:CY:283:PRO:HD3  | 1.96                     | 0.65              |
| 24:CY:312:LEU:HD22 | 24:CY:313:ALA:O    | 1.96                     | 0.65              |
| 29:D4:12:ALA:CB    | 29:D4:29:PRO:HA    | 2.26                     | 0.65              |
| 31:D6:27:LYS:HD2   | 31:D6:30:THR:HB    | 1.78                     | 0.65              |
| 35:DA:2396:G:O2'   | 35:DA:2397:G:H5'   | 1.96                     | 0.65              |
| 35:DA:2408:U:H2'   | 35:DA:2409:G:C8    | 2.32                     | 0.65              |
| 35:DA:2068:U:N3    | 35:DA:2430:A:C2    | 2.63                     | 0.65              |
| 40:DF:65:TRP:CZ3   | 40:DF:75:HIS:HD2   | 2.15                     | 0.65              |
| 48:DP:6:LEU:HB3    | 48:DP:9:ASN:HD21   | 1.59                     | 0.65              |
| 50:DR:87:TYR:C     | 50:DR:89:ASP:H     | 1.99                     | 0.65              |
| 52:DT:88:ILE:HG22  | 52:DT:89:VAL:HG23  | 1.79                     | 0.65              |
| 58:DZ:166:SER:HB2  | 58:DZ:168:GLU:H    | 1.59                     | 0.65              |
| 1:AA:1288:A:N1     | 1:AA:1371:G:H1'    | 2.10                     | 0.65              |
| 1:AA:460:G:H5'     | 1:AA:461:A:OP2     | 1.96                     | 0.65              |
| 4:AD:131:ARG:HD3   | 4:AD:131:ARG:H     | 1.61                     | 0.65              |
| 6:AF:68:PRO:HG2    | 6:AF:71:ARG:HB2    | 1.78                     | 0.65              |
| 16:AP:28:ARG:HG2   | 16:AP:29:ASP:OD2   | 1.97                     | 0.65              |
| 16:AP:43:LYS:HA    | 16:AP:48:TRP:HB3   | 1.77                     | 0.65              |
| 24:AY:192:LEU:O    | 24:AY:192:LEU:HD13 | 1.96                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 35:BA:2497:A:OP2    | 35:BA:2497:A:H8    | 1.80                     | 0.65              |
| 35:BA:613:G:H5'     | 35:BA:613:G:H8     | 1.60                     | 0.65              |
| 37:BC:74:ARG:H      | 37:BC:112:ASP:HB2  | 1.60                     | 0.65              |
| 44:BK:4:VAL:HG12    | 44:BK:5:VAL:N      | 2.05                     | 0.65              |
| 53:BU:107:ALA:HA    | 53:BU:110:VAL:HG23 | 1.79                     | 0.65              |
| 57:BY:8:LYS:HB2     | 57:BY:28:LYS:HZ1   | 1.62                     | 0.65              |
| 1:CA:1346:A:H61     | 1:CA:1374:A:H3'    | 1.61                     | 0.65              |
| 4:CD:129:ASN:HD21   | 4:CD:145:GLU:N     | 1.92                     | 0.65              |
| 10:CJ:4:ILE:HB      | 10:CJ:74:ILE:CG1   | 2.26                     | 0.65              |
| 16:CP:8:ARG:HB3     | 16:CP:28:ARG:NH1   | 2.10                     | 0.65              |
| 24:CY:400:GLU:O     | 24:CY:402:ILE:HD12 | 1.96                     | 0.65              |
| 24:CY:69:VAL:HA     | 24:CY:81:ILE:O     | 1.97                     | 0.65              |
| 24:CY:21:ILE:HG23   | 24:CY:86:GLY:O     | 1.96                     | 0.65              |
| 26:D1:50:ARG:HG2    | 26:D1:57:GLU:OE2   | 1.97                     | 0.65              |
| 35:DA:1142(A):A:O2' | 35:DA:1143:A:H2'   | 1.96                     | 0.65              |
| 35:DA:613:G:H8      | 35:DA:613:G:H5'    | 1.62                     | 0.65              |
| 44:DK:14:ALA:HA     | 44:DK:41:PHE:CE2   | 2.31                     | 0.65              |
| 48:DP:41:ARG:HH21   | 48:DP:41:ARG:CA    | 2.04                     | 0.65              |
| 50:DR:72:ASP:OD1    | 50:DR:75:LEU:HB2   | 1.96                     | 0.65              |
| 3:AC:58:GLU:HB2     | 3:AC:65:ALA:HB2    | 1.78                     | 0.65              |
| 7:AG:80:VAL:HG23    | 7:AG:81:GLY:N      | 2.11                     | 0.65              |
| 21:AU:23:PRO:C      | 21:AU:25:LYS:H     | 2.00                     | 0.65              |
| 26:B1:23:LYS:HD3    | 26:B1:28:GLY:HA3   | 1.77                     | 0.65              |
| 28:B3:36:VAL:O      | 28:B3:37:LEU:HD23  | 1.96                     | 0.65              |
| 19:AS:64:GLU:HG2    | 29:B4:48:ARG:HH22  | 1.59                     | 0.65              |
| 29:B4:56:VAL:O      | 29:B4:57:GLU:HB2   | 1.97                     | 0.65              |
| 30:B5:36:CYS:SG     | 30:B5:48:GLU:O     | 2.52                     | 0.65              |
| 35:BA:2346:A:C2     | 35:BA:2383:G:C2    | 2.85                     | 0.65              |
| 38:BD:186:HIS:HD2   | 38:BD:188:GLU:H    | 1.45                     | 0.65              |
| 40:BF:154:VAL:HG13  | 40:BF:191:ARG:O    | 1.96                     | 0.65              |
| 40:BF:198:ALA:O     | 40:BF:201:VAL:HG12 | 1.96                     | 0.65              |
| 1:CA:973:G:H3'      | 1:CA:974:A:H5''    | 1.79                     | 0.65              |
| 13:CM:108:ARG:HA    | 13:CM:108:ARG:HH11 | 1.60                     | 0.65              |
| 20:CT:82:SER:O      | 20:CT:86:ARG:HB2   | 1.96                     | 0.65              |
| 24:CY:5:VAL:HG13    | 24:CY:6:GLU:N      | 2.12                     | 0.65              |
| 35:DA:1917:U:O2'    | 35:DA:1918:A:H5'   | 1.97                     | 0.65              |
| 35:DA:195:A:H5''    | 35:DA:196:A:OP2    | 1.96                     | 0.65              |
| 35:DA:20:C:O2'      | 35:DA:21:A:H5'     | 1.97                     | 0.65              |
| 38:DD:267:SER:CA    | 38:DD:270:ILE:HD11 | 2.26                     | 0.65              |
| 39:DE:113:PHE:CE2   | 39:DE:158:GLY:HA2  | 2.31                     | 0.65              |
| 1:AA:1328:C:H2'     | 1:AA:1329:A:C8     | 2.32                     | 0.65              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:183:G:H2'     | 1:AA:184:G:C8     | 2.31                     | 0.65              |
| 24:AY:21:ILE:N     | 24:AY:21:ILE:HD13 | 2.11                     | 0.65              |
| 24:AY:334:THR:HG21 | 24:AY:370:LYS:HG2 | 1.79                     | 0.65              |
| 24:AY:637:ARG:HH11 | 24:AY:637:ARG:HG3 | 1.61                     | 0.65              |
| 31:B6:15:GLU:CD    | 31:B6:44:ARG:NH1  | 2.50                     | 0.65              |
| 31:B6:47:THR:HG23  | 31:B6:48:VAL:N    | 2.12                     | 0.65              |
| 31:B6:48:VAL:CG2   | 31:B6:49:HIS:H    | 2.08                     | 0.65              |
| 35:BA:1329:U:H5'   | 35:BA:1330:C:H5   | 1.62                     | 0.65              |
| 35:BA:139:G:C6     | 35:BA:140:G:H2'   | 2.32                     | 0.65              |
| 35:BA:2632:A:N3    | 39:BE:61:ARG:NH1  | 2.45                     | 0.65              |
| 36:BB:15:A:H3'     | 36:BB:16:G:C5'    | 2.25                     | 0.65              |
| 35:BA:84:A:H5'     | 57:BY:9:LYS:HB3   | 1.79                     | 0.65              |
| 1:CA:1328:C:H2'    | 1:CA:1329:A:H8    | 1.61                     | 0.65              |
| 1:CA:1513:A:H2'    | 1:CA:1514:C:C6    | 2.32                     | 0.65              |
| 1:CA:737:A:H2'     | 1:CA:738:C:C6     | 2.32                     | 0.65              |
| 1:CA:773:G:O2'     | 1:CA:774:G:H5'    | 1.97                     | 0.65              |
| 2:CB:22:LYS:H      | 2:CB:40:HIS:HE1   | 1.43                     | 0.65              |
| 4:CD:16:GLY:HA2    | 4:CD:33:MET:HE1   | 1.78                     | 0.65              |
| 12:CL:28:LYS:HE2   | 12:CL:33:ARG:HH12 | 1.62                     | 0.65              |
| 30:D5:20:ARG:HG2   | 30:D5:23:HIS:CD2  | 2.31                     | 0.65              |
| 35:DA:1542:A:H5'   | 35:DA:1543:C:OP2  | 1.95                     | 0.65              |
| 35:DA:1819:A:H4'   | 35:DA:1820:U:H5'  | 1.78                     | 0.65              |
| 35:DA:2196:C:O2'   | 35:DA:2197:U:H5'  | 1.97                     | 0.65              |
| 35:DA:2202:C:H2'   | 38:DD:151:LYS:NZ  | 2.11                     | 0.65              |
| 35:DA:83:G:N2      | 35:DA:102:G:H2'   | 2.12                     | 0.65              |
| 36:DB:48:A:H2'     | 36:DB:49:C:H6     | 1.61                     | 0.65              |
| 37:DC:48:LEU:HD12  | 37:DC:48:LEU:N    | 2.12                     | 0.65              |
| 44:DK:103:GLN:O    | 44:DK:106:GLU:HG2 | 1.97                     | 0.65              |
| 35:DA:666:G:H4'    | 48:DP:49:ARG:HH21 | 1.62                     | 0.65              |
| 1:AA:270:A:H2'     | 1:AA:271:C:C6     | 2.32                     | 0.65              |
| 24:AY:21:ILE:CG2   | 24:AY:88:VAL:HG13 | 2.27                     | 0.65              |
| 35:BA:1345:C:O2'   | 35:BA:1346:G:H5'  | 1.97                     | 0.65              |
| 35:BA:1514:U:H2'   | 35:BA:1515:G:C8   | 2.32                     | 0.65              |
| 35:BA:2462:U:H2'   | 35:BA:2463:C:H6   | 1.61                     | 0.65              |
| 40:BF:132:VAL:HG22 | 40:BF:133:ASN:H   | 1.62                     | 0.65              |
| 51:BS:89:ARG:HH11  | 51:BS:89:ARG:HG2  | 1.62                     | 0.65              |
| 52:BT:33:LYS:HE2   | 52:BT:43:GLN:OE1  | 1.97                     | 0.65              |
| 52:BT:24:PRO:HD3   | 52:BT:52:ILE:CD1  | 2.27                     | 0.65              |
| 56:BX:70:LEU:HD23  | 56:BX:71:GLY:N    | 2.12                     | 0.65              |
| 58:BZ:115:GLY:CA   | 58:BZ:177:PRO:HG3 | 2.26                     | 0.65              |
| 1:CA:1104:G:O5'    | 2:CB:111:ARG:HD2  | 1.96                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:CM:90:LEU:O     | 13:CM:92:HIS:N     | 2.30                     | 0.65              |
| 16:CP:8:ARG:HB3    | 16:CP:28:ARG:HH12  | 1.62                     | 0.65              |
| 24:CY:496:LYS:HE2  | 24:CY:498:ILE:HD13 | 1.78                     | 0.65              |
| 33:D8:13:ARG:HH12  | 48:DP:59:LEU:HG    | 1.60                     | 0.65              |
| 35:DA:1127:A:H2'   | 35:DA:1128:A:H5''  | 1.79                     | 0.65              |
| 35:DA:2241:A:H2'   | 35:DA:2242:G:H8    | 1.62                     | 0.65              |
| 35:DA:936:C:H2'    | 35:DA:937:U:C6     | 2.32                     | 0.65              |
| 38:DD:148:GLU:HB2  | 38:DD:151:LYS:HG3  | 1.79                     | 0.65              |
| 41:DG:55:LYS:HA    | 41:DG:58:GLN:HG3   | 1.78                     | 0.65              |
| 50:DR:45:ARG:HG3   | 50:DR:46:GLY:N     | 2.11                     | 0.65              |
| 52:DT:82:LEU:HD12  | 52:DT:82:LEU:N     | 2.11                     | 0.65              |
| 1:AA:1211:U:H5'    | 1:AA:1212:U:OP1    | 1.97                     | 0.65              |
| 1:AA:163:C:O2'     | 1:AA:164:U:H5'     | 1.97                     | 0.65              |
| 3:AC:105:GLU:HG2   | 3:AC:106:VAL:H     | 1.62                     | 0.65              |
| 11:AK:33:THR:HA    | 11:AK:40:ILE:HG12  | 1.79                     | 0.65              |
| 13:AM:4:ILE:HG22   | 13:AM:5:ALA:H      | 1.62                     | 0.65              |
| 1:AA:1305:G:OP1    | 21:AU:2:GLY:N      | 2.30                     | 0.65              |
| 24:AY:530:VAL:HG22 | 24:AY:531:GLY:N    | 2.11                     | 0.65              |
| 35:BA:1183:G:O2'   | 35:BA:1184:G:H5'   | 1.96                     | 0.65              |
| 35:BA:2039:C:H2'   | 35:BA:2040:C:C6    | 2.32                     | 0.65              |
| 35:BA:2832:U:H1'   | 35:BA:2834:G:N3    | 2.12                     | 0.65              |
| 35:BA:2855:C:H2'   | 35:BA:2856:C:H6    | 1.63                     | 0.65              |
| 35:BA:564:C:O2'    | 35:BA:565:C:H5'    | 1.97                     | 0.65              |
| 39:BE:11:MET:HB3   | 39:BE:24:THR:HA    | 1.79                     | 0.65              |
| 44:BK:19:PRO:CB    | 44:BK:34:ILE:HD12  | 2.23                     | 0.65              |
| 35:BA:1012:U:C5    | 46:BN:28:THR:HG21  | 2.32                     | 0.65              |
| 53:BU:68:ALA:O     | 53:BU:71:GLN:HB3   | 1.96                     | 0.65              |
| 57:BY:88:LYS:O     | 57:BY:90:LEU:HD23  | 1.97                     | 0.65              |
| 1:CA:1288:A:N1     | 1:CA:1371:G:H1'    | 2.12                     | 0.65              |
| 1:CA:687:A:N6      | 1:CA:703:G:H1'     | 2.12                     | 0.65              |
| 1:CA:715:A:H2'     | 1:CA:716:A:C8      | 2.32                     | 0.65              |
| 8:CH:103:VAL:CG2   | 8:CH:110:ALA:HB2   | 2.27                     | 0.65              |
| 26:D1:8:SER:HB3    | 26:D1:66:HIS:CD2   | 2.32                     | 0.65              |
| 35:DA:1217:C:OP2   | 53:DU:15:LYS:NZ    | 2.23                     | 0.65              |
| 35:DA:1946:U:H2'   | 35:DA:1947:C:H6    | 1.60                     | 0.65              |
| 35:DA:2162:G:H2'   | 35:DA:2163:C:C6    | 2.32                     | 0.65              |
| 35:DA:2345:G:C5'   | 35:DA:2346:A:H5'   | 2.27                     | 0.65              |
| 35:DA:2455:G:H2'   | 35:DA:2456:C:C6    | 2.31                     | 0.65              |
| 35:DA:2537:U:H2'   | 35:DA:2538:C:C6    | 2.32                     | 0.65              |
| 35:DA:272(B):G:H2' | 35:DA:272(C):G:H8  | 1.62                     | 0.65              |
| 35:DA:295:G:H2'    | 35:DA:296:C:H6     | 1.62                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:422:A:H2'    | 35:DA:423:A:C8     | 2.32                     | 0.65              |
| 35:DA:796:C:H2'    | 35:DA:797:C:C6     | 2.31                     | 0.65              |
| 41:DG:40:ASN:HD22  | 41:DG:41:GLN:H     | 1.45                     | 0.65              |
| 2:AB:220:ASP:O     | 2:AB:223:ILE:HG13  | 1.98                     | 0.64              |
| 11:AK:85:ARG:HG2   | 11:AK:111:ASP:O    | 1.97                     | 0.64              |
| 11:AK:48:ILE:HG22  | 11:AK:49:GLY:H     | 1.61                     | 0.64              |
| 18:AR:31:LEU:H     | 18:AR:31:LEU:CD2   | 2.10                     | 0.64              |
| 24:AY:342:TYR:CE2  | 24:AY:396:ARG:HD2  | 2.31                     | 0.64              |
| 24:AY:434:GLU:OE1  | 24:AY:465:ARG:NH2  | 2.30                     | 0.64              |
| 24:AY:628:ARG:NH1  | 24:AY:680:PRO:HG2  | 2.12                     | 0.64              |
| 26:B1:76:ARG:HH22  | 26:B1:95:LEU:HD13  | 1.62                     | 0.64              |
| 22:AW:66:C:H4'     | 31:B6:28:ARG:HH22  | 1.61                     | 0.64              |
| 35:BA:1052:C:H2'   | 35:BA:1053:C:C6    | 2.31                     | 0.64              |
| 35:BA:1657:C:O2'   | 35:BA:1658:C:H5'   | 1.97                     | 0.64              |
| 35:BA:2815:C:H2'   | 35:BA:2816:C:C6    | 2.32                     | 0.64              |
| 35:BA:284:U:H2'    | 35:BA:285:C:H6     | 1.63                     | 0.64              |
| 41:BG:82:LEU:CD1   | 41:BG:87:PRO:HB3   | 2.28                     | 0.64              |
| 35:BA:1029:A:H5''  | 49:BQ:128:LYS:HE3  | 1.79                     | 0.64              |
| 49:BQ:97:VAL:HG11  | 49:BQ:103:MET:CE   | 2.26                     | 0.64              |
| 51:BS:19:LYS:HB3   | 51:BS:20:ARG:HH22  | 1.60                     | 0.64              |
| 56:BX:30:VAL:HG22  | 56:BX:77:LYS:O     | 1.97                     | 0.64              |
| 1:CA:942:G:H21     | 9:CI:124:GLN:HE22  | 1.43                     | 0.64              |
| 4:CD:33:MET:O      | 4:CD:37:PRO:HG3    | 1.95                     | 0.64              |
| 5:CE:72:GLN:HE22   | 5:CE:144:THR:HG22  | 1.62                     | 0.64              |
| 19:CS:58:VAL:HG23  | 19:CS:58:VAL:O     | 1.97                     | 0.64              |
| 22:CV:59:A:H2'     | 22:CV:60:U:H5'     | 1.79                     | 0.64              |
| 24:CY:227:ILE:HD12 | 24:CY:245:ALA:HB2  | 1.78                     | 0.64              |
| 31:D6:47:THR:HG23  | 31:D6:48:VAL:N     | 2.12                     | 0.64              |
| 35:DA:1514:U:H2'   | 35:DA:1515:G:C8    | 2.32                     | 0.64              |
| 35:DA:221:A:H61    | 35:DA:265:A:H8     | 1.43                     | 0.64              |
| 35:DA:2347:C:H2'   | 35:DA:2348:U:C6    | 2.31                     | 0.64              |
| 35:DA:419:C:H2'    | 35:DA:420:C:C6     | 2.32                     | 0.64              |
| 39:DE:131:ALA:CB   | 39:DE:134:ILE:HD11 | 2.14                     | 0.64              |
| 35:DA:2312:U:O2'   | 41:DG:71:THR:HG21  | 1.98                     | 0.64              |
| 56:DX:41:ASN:C     | 56:DX:43:VAL:H     | 2.00                     | 0.64              |
| 1:AA:1310:G:O2'    | 1:AA:1311:G:H5'    | 1.97                     | 0.64              |
| 1:AA:999:C:H2'     | 1:AA:1000:U:C5     | 2.32                     | 0.64              |
| 3:AC:178:LEU:O     | 3:AC:180:ALA:N     | 2.30                     | 0.64              |
| 20:AT:43:LEU:O     | 20:AT:46:GLU:N     | 2.30                     | 0.64              |
| 22:AV:17:C:C6      | 22:AV:17(A):U:H5   | 2.15                     | 0.64              |
| 35:BA:267:C:H2'    | 35:BA:268:C:H6     | 1.63                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BB:48:A:H2'     | 36:BB:49:C:H6      | 1.61                     | 0.64              |
| 36:BB:50:G:OP1     | 51:BS:63:THR:HG23  | 1.97                     | 0.64              |
| 37:BC:176:VAL:HG21 | 37:BC:190:ILE:CD1  | 2.27                     | 0.64              |
| 38:BD:267:SER:O    | 38:BD:269:PHE:N    | 2.29                     | 0.64              |
| 38:BD:39:LYS:NZ    | 38:BD:87:ASN:HB3   | 2.13                     | 0.64              |
| 38:BD:43:ARG:HB3   | 38:BD:54:ARG:HB2   | 1.79                     | 0.64              |
| 41:BG:68:PRO:CB    | 41:BG:90:LEU:HD11  | 2.26                     | 0.64              |
| 49:BQ:56:ARG:HA    | 49:BQ:56:ARG:HE    | 1.62                     | 0.64              |
| 49:BQ:75:THR:HG22  | 49:BQ:76:LYS:N     | 2.11                     | 0.64              |
| 52:BT:55:ASN:H     | 52:BT:59:THR:CG2   | 2.10                     | 0.64              |
| 55:BW:64:MET:O     | 55:BW:65:LEU:HB3   | 1.96                     | 0.64              |
| 1:CA:1248:A:C2'    | 1:CA:1249:C:H5'    | 2.26                     | 0.64              |
| 4:CD:30:LYS:O      | 4:CD:32:ALA:N      | 2.30                     | 0.64              |
| 5:CE:78:HIS:O      | 5:CE:93:PRO:HD3    | 1.97                     | 0.64              |
| 14:CN:16:PHE:N     | 14:CN:16:PHE:CD1   | 2.61                     | 0.64              |
| 16:CP:43:LYS:HA    | 16:CP:48:TRP:HB3   | 1.78                     | 0.64              |
| 21:CU:23:PRO:C     | 21:CU:25:LYS:H     | 2.00                     | 0.64              |
| 33:D8:50:LEU:HD12  | 33:D8:51:ALA:N     | 2.12                     | 0.64              |
| 33:D8:50:LEU:CD1   | 33:D8:51:ALA:H     | 2.08                     | 0.64              |
| 35:DA:2205:C:H5'   | 35:DA:2206:G:OP2   | 1.98                     | 0.64              |
| 35:DA:2591:C:H2'   | 35:DA:2592:G:H8    | 1.62                     | 0.64              |
| 35:DA:2632:A:N3    | 39:DE:61:ARG:NH1   | 2.46                     | 0.64              |
| 35:DA:272(H):C:H2' | 35:DA:272(I):U:C5' | 2.28                     | 0.64              |
| 35:DA:2762:G:H5'   | 35:DA:2762:G:C8    | 2.32                     | 0.64              |
| 38:DD:232:PRO:HD2  | 38:DD:249:PRO:HA   | 1.80                     | 0.64              |
| 40:DF:123:LEU:HD12 | 40:DF:124:LEU:N    | 2.12                     | 0.64              |
| 41:DG:152:LEU:H    | 41:DG:152:LEU:HD23 | 1.63                     | 0.64              |
| 46:DN:46:VAL:O     | 46:DN:47:ALA:CB    | 2.44                     | 0.64              |
| 46:DN:67:LEU:HB3   | 46:DN:88:GLU:CG    | 2.28                     | 0.64              |
| 55:DW:107:LEU:H    | 55:DW:107:LEU:HD22 | 1.62                     | 0.64              |
| 58:DZ:70:LEU:HG    | 58:DZ:91:LEU:HD11  | 1.79                     | 0.64              |
| 1:AA:1218:C:H2'    | 1:AA:1219:U:C6     | 2.33                     | 0.64              |
| 1:AA:1319:A:OP1    | 19:AS:10:PHE:CE1   | 2.50                     | 0.64              |
| 1:AA:1525:G:H2'    | 1:AA:1526:G:H8     | 1.61                     | 0.64              |
| 35:BA:195:A:H5''   | 35:BA:196:A:OP2    | 1.98                     | 0.64              |
| 35:BA:2329:G:H2'   | 35:BA:2330:G:C8    | 2.31                     | 0.64              |
| 35:BA:580:C:H2'    | 35:BA:581:C:C6     | 2.31                     | 0.64              |
| 35:BA:666:G:H4'    | 48:BP:49:ARG:HH21  | 1.59                     | 0.64              |
| 42:BH:156:ALA:O    | 42:BH:158:HIS:N    | 2.30                     | 0.64              |
| 50:BR:87:TYR:C     | 50:BR:89:ASP:H     | 1.99                     | 0.64              |
| 36:BB:115:G:O4'    | 51:BS:47:THR:HB    | 1.98                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 57:BY:97:ARG:HG3  | 57:BY:97:ARG:HH11  | 1.62                     | 0.64              |
| 1:CA:1334:G:H5'   | 1:CA:1335:C:OP2    | 1.98                     | 0.64              |
| 1:CA:382:A:H2'    | 1:CA:383:A:H8      | 1.61                     | 0.64              |
| 4:CD:13:ARG:HA    | 4:CD:33:MET:CE     | 2.27                     | 0.64              |
| 11:CK:48:ILE:HD13 | 11:CK:48:ILE:N     | 2.12                     | 0.64              |
| 12:CL:27:LEU:HD21 | 12:CL:64:TYR:CE1   | 2.32                     | 0.64              |
| 31:D6:48:VAL:CG2  | 31:D6:49:HIS:H     | 2.09                     | 0.64              |
| 32:D7:46:VAL:HG12 | 32:D7:47:ARG:N     | 2.12                     | 0.64              |
| 35:DA:2168:G:N2   | 35:DA:2170:A:H3'   | 2.12                     | 0.64              |
| 35:DA:2344:U:O2'  | 35:DA:2345:G:H5''  | 1.97                     | 0.64              |
| 35:DA:2472:G:H3'  | 35:DA:2475:C:H42   | 1.63                     | 0.64              |
| 35:DA:301:G:H1'   | 35:DA:302:C:C6     | 2.32                     | 0.64              |
| 49:DQ:29:PHE:HB2  | 49:DQ:105:GLU:OE2  | 1.97                     | 0.64              |
| 51:DS:97:ARG:HE   | 51:DS:97:ARG:C     | 2.01                     | 0.64              |
| 52:DT:80:SER:CB   | 52:DT:81:PRO:HD3   | 2.26                     | 0.64              |
| 1:AA:20:U:H2'     | 1:AA:21:G:O4'      | 1.97                     | 0.64              |
| 1:AA:666:G:H5'    | 1:AA:726:C:H1'     | 1.79                     | 0.64              |
| 3:AC:52:LEU:CD2   | 3:AC:52:LEU:H      | 2.09                     | 0.64              |
| 24:AY:276:VAL:CA  | 24:AY:280:LEU:HD23 | 2.24                     | 0.64              |
| 24:AY:343:ASN:ND2 | 24:AY:345:THR:H    | 1.95                     | 0.64              |
| 30:B5:4:HIS:HB3   | 30:B5:5:PRO:CD     | 2.27                     | 0.64              |
| 34:B9:17:ILE:HG21 | 34:B9:19:ARG:HH21  | 1.61                     | 0.64              |
| 35:BA:1380:G:O2'  | 35:BA:1381:G:H5'   | 1.98                     | 0.64              |
| 35:BA:2172:U:H1'  | 35:BA:2173:A:OP1   | 1.97                     | 0.64              |
| 35:BA:2205:C:H5'  | 35:BA:2206:G:OP2   | 1.97                     | 0.64              |
| 35:BA:2408:U:H2'  | 35:BA:2409:G:C8    | 2.32                     | 0.64              |
| 35:BA:83:G:N2     | 35:BA:102:G:H2'    | 2.13                     | 0.64              |
| 36:BB:65:C:H41    | 36:BB:109:C:H2'    | 1.61                     | 0.64              |
| 37:BC:29:LEU:HD23 | 37:BC:29:LEU:C     | 2.17                     | 0.64              |
| 41:BG:42:GLY:HA2  | 41:BG:89:GLY:HA2   | 1.79                     | 0.64              |
| 41:BG:76:SER:HB3  | 41:BG:83:ARG:HB3   | 1.78                     | 0.64              |
| 42:BH:92:ILE:O    | 42:BH:94:TYR:N     | 2.28                     | 0.64              |
| 49:BQ:76:LYS:HB3  | 49:BQ:91:GLU:HG3   | 1.79                     | 0.64              |
| 57:BY:27:VAL:HG12 | 57:BY:29:GLU:H     | 1.59                     | 0.64              |
| 2:CB:14:GLY:O     | 2:CB:15:VAL:HG13   | 1.98                     | 0.64              |
| 2:CB:80:ILE:H     | 2:CB:80:ILE:HD12   | 1.61                     | 0.64              |
| 4:CD:102:ASP:HB3  | 4:CD:136:PRO:HB3   | 1.79                     | 0.64              |
| 5:CE:144:THR:O    | 5:CE:148:VAL:HG23  | 1.97                     | 0.64              |
| 5:CE:20:GLN:O     | 5:CE:21:ALA:C      | 2.36                     | 0.64              |
| 23:CX:15:A:H5'    | 23:CX:16:A:OP1     | 1.98                     | 0.64              |
| 24:CY:612:THR:C   | 24:CY:640:ALA:HB1  | 2.17                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:D6:16:CYS:SG    | 31:D6:48:VAL:CG2   | 2.85                     | 0.64              |
| 35:DA:2573:C:H2'   | 35:DA:2573:C:O2    | 1.96                     | 0.64              |
| 35:DA:629:G:H5''   | 35:DA:650:C:O2'    | 1.96                     | 0.64              |
| 35:DA:723:G:H2'    | 35:DA:724:U:C6     | 2.32                     | 0.64              |
| 38:DD:130:ALA:C    | 38:DD:131:LEU:HD12 | 2.17                     | 0.64              |
| 38:DD:76:PRO:O     | 38:DD:98:VAL:HG23  | 1.97                     | 0.64              |
| 39:DE:199:ARG:HB3  | 39:DE:200:GLU:OE2  | 1.98                     | 0.64              |
| 39:DE:7:VAL:HG12   | 39:DE:27:LEU:HB3   | 1.80                     | 0.64              |
| 39:DE:4:ILE:CD1    | 39:DE:28:ALA:HB1   | 2.27                     | 0.64              |
| 44:DK:78:ILE:HD11  | 44:DK:136:VAL:HG11 | 1.79                     | 0.64              |
| 35:DA:1012:U:C5    | 46:DN:28:THR:HG21  | 2.32                     | 0.64              |
| 48:DP:41:ARG:NH2   | 48:DP:41:ARG:HA    | 2.06                     | 0.64              |
| 53:DU:20:LEU:N     | 53:DU:20:LEU:HD22  | 2.10                     | 0.64              |
| 58:DZ:153:SER:HB2  | 58:DZ:163:LEU:HD13 | 1.79                     | 0.64              |
| 1:AA:1068:G:OP2    | 1:AA:1094:G:H5'    | 1.97                     | 0.64              |
| 1:AA:1284:C:H3'    | 1:AA:1285:A:C5'    | 2.27                     | 0.64              |
| 5:AE:7:GLU:HG2     | 5:AE:112:LEU:CD2   | 2.28                     | 0.64              |
| 13:AM:90:LEU:O     | 13:AM:92:HIS:N     | 2.31                     | 0.64              |
| 19:AS:24:ALA:O     | 19:AS:25:LYS:HB2   | 1.98                     | 0.64              |
| 24:AY:485:GLU:HB2  | 24:AY:560:VAL:HG22 | 1.80                     | 0.64              |
| 29:B4:42:PHE:CD1   | 29:B4:42:PHE:N     | 2.65                     | 0.64              |
| 29:B4:5:ILE:O      | 29:B4:5:ILE:HG12   | 1.96                     | 0.64              |
| 35:BA:1231:G:H2'   | 35:BA:1232:G:H8    | 1.62                     | 0.64              |
| 35:BA:1812:A:H2'   | 35:BA:1813:G:H8    | 1.62                     | 0.64              |
| 35:BA:2348:U:C2'   | 35:BA:2349:G:H5''  | 2.27                     | 0.64              |
| 35:BA:272(H):C:H2' | 35:BA:272(I):U:C5' | 2.27                     | 0.64              |
| 47:BO:18:LYS:HB2   | 47:BO:45:GLU:HG2   | 1.80                     | 0.64              |
| 35:BA:2392:A:C8    | 48:BP:60:MET:HB3   | 2.31                     | 0.64              |
| 58:BZ:115:GLY:N    | 58:BZ:177:PRO:CG   | 2.60                     | 0.64              |
| 58:BZ:41:LEU:O     | 58:BZ:44:PHE:N     | 2.30                     | 0.64              |
| 1:CA:194:C:C2'     | 1:CA:195:A:H5''    | 2.27                     | 0.64              |
| 9:CI:8:GLY:HA2     | 9:CI:79:LEU:HD12   | 1.78                     | 0.64              |
| 11:CK:33:THR:HA    | 11:CK:40:ILE:HG12  | 1.80                     | 0.64              |
| 12:CL:28:LYS:HE2   | 12:CL:33:ARG:NH1   | 2.13                     | 0.64              |
| 16:CP:14:ASN:N     | 16:CP:15:PRO:HD3   | 2.13                     | 0.64              |
| 20:CT:50:GLU:HB3   | 20:CT:99:LEU:HB2   | 1.80                     | 0.64              |
| 24:CY:198:GLU:HG3  | 24:CY:198:GLU:O    | 1.97                     | 0.64              |
| 24:CY:539:ILE:HA   | 24:CY:542:VAL:HG12 | 1.79                     | 0.64              |
| 30:D5:36:CYS:SG    | 30:D5:48:GLU:O     | 2.55                     | 0.64              |
| 31:D6:6:ARG:HD2    | 31:D6:6:ARG:H      | 1.62                     | 0.64              |
| 35:DA:1223:G:H5'   | 35:DA:1224:C:OP2   | 1.98                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:1814:G:C3'   | 35:DA:1815:A:H5''  | 2.27                     | 0.64              |
| 35:DA:2228:G:H2'   | 35:DA:2229:C:C6    | 2.33                     | 0.64              |
| 40:DF:25:PRO:HG3   | 40:DF:119:ARG:HB2  | 1.79                     | 0.64              |
| 41:DG:111:LEU:HD23 | 41:DG:114:ILE:HD11 | 1.79                     | 0.64              |
| 48:DP:115:LEU:HD23 | 48:DP:115:LEU:N    | 2.13                     | 0.64              |
| 33:D8:25:MET:HG3   | 48:DP:64:LYS:HB2   | 1.79                     | 0.64              |
| 57:DY:51:VAL:C     | 57:DY:53:PRO:HD2   | 2.17                     | 0.64              |
| 58:DZ:10:ARG:HB3   | 58:DZ:36:LYS:HB2   | 1.80                     | 0.64              |
| 58:DZ:40:ASP:OD1   | 58:DZ:42:VAL:HG12  | 1.96                     | 0.64              |
| 1:AA:1489:G:C3'    | 1:AA:1490:C:H5''   | 2.27                     | 0.64              |
| 1:AA:477:A:O2'     | 1:AA:479:C:H5'     | 1.98                     | 0.64              |
| 1:AA:980:C:C5      | 1:AA:981:U:C2      | 2.84                     | 0.64              |
| 4:AD:121:VAL:O     | 4:AD:134:ASP:HA    | 1.97                     | 0.64              |
| 4:AD:88:VAL:O      | 4:AD:92:VAL:HG23   | 1.98                     | 0.64              |
| 20:AT:13:LEU:HD12  | 20:AT:13:LEU:N     | 2.10                     | 0.64              |
| 22:AV:6:G:H1       | 22:AV:67:C:H42     | 1.44                     | 0.64              |
| 24:AY:20:HIS:HB2   | 24:AY:87:HIS:HD2   | 1.61                     | 0.64              |
| 31:B6:43:CYS:O     | 31:B6:44:ARG:HB2   | 1.97                     | 0.64              |
| 35:BA:1362:C:O2'   | 35:BA:1363:C:H5'   | 1.98                     | 0.64              |
| 35:BA:2523:G:H2'   | 35:BA:2524:G:C5'   | 2.24                     | 0.64              |
| 35:BA:392:C:H5''   | 35:BA:409:C:H5''   | 1.80                     | 0.64              |
| 29:B4:2:LYS:HG2    | 36:BB:44:G:OP2     | 1.98                     | 0.64              |
| 36:BB:92:C:H2'     | 36:BB:93:G:H8      | 1.62                     | 0.64              |
| 51:BS:59:LYS:HD2   | 51:BS:61:ASN:HB2   | 1.79                     | 0.64              |
| 51:BS:97:ARG:HH21  | 51:BS:98:VAL:HA    | 1.62                     | 0.64              |
| 52:BT:24:PRO:HD3   | 52:BT:52:ILE:HD11  | 1.79                     | 0.64              |
| 44:BK:93:ARG:HB2   | 58:BZ:112:ARG:NH2  | 2.12                     | 0.64              |
| 1:CA:41:G:H2'      | 1:CA:42:G:C8       | 2.33                     | 0.64              |
| 3:CC:105:GLU:HG2   | 3:CC:106:VAL:H     | 1.62                     | 0.64              |
| 3:CC:136:GLN:HG3   | 3:CC:139:GLN:HB3   | 1.79                     | 0.64              |
| 18:CR:31:LEU:H     | 18:CR:31:LEU:CD2   | 2.10                     | 0.64              |
| 26:D1:8:SER:HB3    | 26:D1:66:HIS:NE2   | 2.13                     | 0.64              |
| 28:D3:15:TYR:HB3   | 28:D3:19:GLN:NE2   | 2.13                     | 0.64              |
| 29:D4:42:PHE:N     | 29:D4:42:PHE:CD1   | 2.66                     | 0.64              |
| 35:DA:1012:U:H3    | 46:DN:25:ARG:HE    | 1.46                     | 0.64              |
| 1:AA:559:A:H4'     | 1:AA:560:U:C5'     | 2.27                     | 0.64              |
| 1:AA:72:C:H2'      | 1:AA:73:G:H8       | 1.63                     | 0.64              |
| 5:AE:6:PHE:HB3     | 5:AE:35:GLY:O      | 1.98                     | 0.64              |
| 19:AS:40:ILE:HG21  | 19:AS:66:MET:O     | 1.97                     | 0.64              |
| 35:BA:1036:G:OP1   | 42:BH:59:ARG:HD2   | 1.96                     | 0.64              |
| 35:BA:1053:C:H3'   | 35:BA:1054:A:H5''  | 1.79                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:2442:C:H2'   | 35:BA:2443:C:H6    | 1.63                     | 0.64              |
| 47:BO:24:VAL:CG2   | 47:BO:30:ALA:HB3   | 2.27                     | 0.64              |
| 47:BO:104:ARG:HH21 | 52:BT:33:LYS:CE    | 2.11                     | 0.64              |
| 58:BZ:109:ALA:C    | 58:BZ:111:VAL:H    | 1.98                     | 0.64              |
| 24:CY:438:PHE:HD2  | 24:CY:438:PHE:C    | 2.01                     | 0.64              |
| 35:DA:1038:C:C3'   | 35:DA:1039:G:H5''  | 2.26                     | 0.64              |
| 35:DA:1438:U:O2'   | 35:DA:1439:A:H5'   | 1.97                     | 0.64              |
| 35:DA:1902:C:H4'   | 38:DD:244:ARG:HB2  | 1.79                     | 0.64              |
| 35:DA:2186:G:C2'   | 35:DA:2187:G:H5''  | 2.27                     | 0.64              |
| 31:D6:5:VAL:CG2    | 35:DA:2283:C:H5'   | 2.22                     | 0.64              |
| 35:DA:272(J):C:C3' | 35:DA:274:G:H5''   | 2.25                     | 0.64              |
| 35:DA:2815:C:H2'   | 35:DA:2816:C:C6    | 2.32                     | 0.64              |
| 35:DA:781:A:C8     | 38:DD:219:PRO:HG3  | 2.33                     | 0.64              |
| 36:DB:65:C:H41     | 36:DB:109:C:H2'    | 1.61                     | 0.64              |
| 38:DD:158:ALA:HB3  | 38:DD:161:THR:CG2  | 2.25                     | 0.64              |
| 40:DF:4:VAL:HG22   | 40:DF:19:GLU:OE1   | 1.97                     | 0.64              |
| 40:DF:78:ILE:HA    | 40:DF:83:PHE:CD1   | 2.33                     | 0.64              |
| 41:DG:40:ASN:HD22  | 41:DG:41:GLN:N     | 1.94                     | 0.64              |
| 44:DK:41:PHE:CE1   | 44:DK:45:THR:HG21  | 2.32                     | 0.64              |
| 46:DN:58:ASP:OD2   | 46:DN:59:LYS:HG2   | 1.96                     | 0.64              |
| 50:DR:117:VAL:HG12 | 50:DR:118:GLU:N    | 2.12                     | 0.64              |
| 52:DT:132:LYS:HD3  | 52:DT:132:LYS:N    | 2.13                     | 0.64              |
| 1:AA:1320:C:OP1    | 19:AS:70:LYS:NZ    | 2.31                     | 0.64              |
| 2:AB:140:HIS:O     | 2:AB:143:GLU:HB2   | 1.96                     | 0.64              |
| 4:AD:16:GLY:HA2    | 4:AD:33:MET:CE     | 2.28                     | 0.64              |
| 16:AP:50:LYS:HG2   | 16:AP:51:VAL:N     | 2.12                     | 0.64              |
| 24:AY:534:ILE:HD12 | 24:AY:567:LEU:HD11 | 1.80                     | 0.64              |
| 27:B2:64:LEU:HD22  | 27:B2:64:LEU:O     | 1.98                     | 0.64              |
| 35:BA:145:G:H2'    | 35:BA:146:G:H8     | 1.63                     | 0.64              |
| 35:BA:1514:U:H2'   | 35:BA:1515:G:H8    | 1.63                     | 0.64              |
| 35:BA:1718:G:H8    | 35:BA:1718:G:H5'   | 1.62                     | 0.64              |
| 35:BA:814:C:H2'    | 35:BA:815:C:C6     | 2.31                     | 0.64              |
| 38:BD:117:VAL:HG23 | 38:BD:129:ASN:HA   | 1.79                     | 0.64              |
| 39:BE:4:ILE:CD1    | 39:BE:28:ALA:HB1   | 2.27                     | 0.64              |
| 40:BF:123:LEU:HD13 | 40:BF:192:LEU:HD22 | 1.79                     | 0.64              |
| 41:BG:34:LEU:HB2   | 41:BG:99:MET:HE1   | 1.79                     | 0.64              |
| 48:BP:6:LEU:HB3    | 48:BP:9:ASN:HD21   | 1.61                     | 0.64              |
| 51:BS:66:ALA:O     | 51:BS:99:LYS:HA    | 1.98                     | 0.64              |
| 1:AA:346:G:OP1     | 52:BT:41:ARG:NH2   | 2.31                     | 0.64              |
| 52:BT:88:ILE:HG22  | 52:BT:89:VAL:HG23  | 1.79                     | 0.64              |
| 1:CA:1006:C:H2'    | 1:CA:1007:C:C6     | 2.32                     | 0.64              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:188:C:H2'    | 1:CA:189:G:H8      | 1.62                     | 0.64              |
| 1:CA:60:A:H5''    | 1:CA:331:G:N2      | 2.13                     | 0.64              |
| 1:CA:54:C:H2'     | 1:CA:352:C:H41     | 1.63                     | 0.64              |
| 12:CL:69:TYR:O    | 12:CL:71:PRO:HD3   | 1.98                     | 0.64              |
| 13:CM:10:PRO:CB   | 13:CM:18:ALA:HB1   | 2.27                     | 0.64              |
| 20:CT:43:LEU:HB3  | 20:CT:48:LYS:HB2   | 1.80                     | 0.64              |
| 24:CY:104:ALA:O   | 24:CY:132:ARG:HB2  | 1.98                     | 0.64              |
| 61:CY:702:FUA:C23 | 61:CY:702:FUA:H122 | 2.28                     | 0.64              |
| 27:D2:33:MET:SD   | 56:DX:5:TYR:HD2    | 2.21                     | 0.64              |
| 31:D6:43:CYS:O    | 31:D6:44:ARG:HB2   | 1.97                     | 0.64              |
| 31:D6:45:LYS:HG2  | 35:DA:2371:G:H4'   | 1.80                     | 0.64              |
| 35:DA:2497:A:OP2  | 35:DA:2497:A:H8    | 1.80                     | 0.64              |
| 35:DA:322:A:OP2   | 40:DF:169:ASN:HB2  | 1.98                     | 0.64              |
| 25:D0:26:TYR:HE2  | 35:DA:857:C:H1'    | 1.63                     | 0.64              |
| 38:DD:24:ILE:HD13 | 38:DD:25:THR:N     | 2.11                     | 0.64              |
| 40:DF:16:GLY:O    | 40:DF:17:ARG:HG3   | 1.98                     | 0.64              |
| 40:DF:198:ALA:O   | 40:DF:201:VAL:HG12 | 1.97                     | 0.64              |
| 46:DN:3:THR:HG22  | 46:DN:4:TYR:N      | 2.11                     | 0.64              |
| 57:DY:95:LYS:HD3  | 57:DY:100:ALA:HB1  | 1.79                     | 0.64              |
| 1:AA:176:C:H2'    | 1:AA:177:C:C6      | 2.32                     | 0.64              |
| 24:AY:9:LEU:CD2   | 24:AY:284:LEU:HB2  | 2.25                     | 0.64              |
| 61:AY:702:FUA:C20 | 61:AY:702:FUA:H5   | 2.12                     | 0.64              |
| 28:B3:15:TYR:HB3  | 28:B3:19:GLN:NE2   | 2.13                     | 0.64              |
| 35:BA:1237:A:O2'  | 35:BA:1238:G:O4'   | 2.16                     | 0.64              |
| 35:BA:1538:G:H2'  | 35:BA:1539:G:H8    | 1.60                     | 0.64              |
| 35:BA:2248:C:C2'  | 35:BA:2249:U:H5'   | 2.28                     | 0.64              |
| 35:BA:2750:A:H2'  | 35:BA:2752:C:H41   | 1.62                     | 0.64              |
| 37:BC:28:ARG:NH1  | 37:BC:183:PRO:HB2  | 2.12                     | 0.64              |
| 38:BD:10:THR:HG23 | 38:BD:13:ARG:HB3   | 1.79                     | 0.64              |
| 41:BG:98:ARG:N    | 41:BG:98:ARG:HH11  | 1.95                     | 0.64              |
| 42:BH:137:ASP:HB3 | 42:BH:140:LYS:HB2  | 1.78                     | 0.64              |
| 44:BK:6:ALA:O     | 44:BK:58:THR:HG23  | 1.97                     | 0.64              |
| 44:BK:77:LEU:N    | 44:BK:77:LEU:HD23  | 2.11                     | 0.64              |
| 49:BQ:56:ARG:HA   | 49:BQ:56:ARG:NE    | 2.13                     | 0.64              |
| 52:BT:132:LYS:N   | 52:BT:132:LYS:HD3  | 2.12                     | 0.64              |
| 57:BY:51:VAL:HG12 | 57:BY:53:PRO:HD2   | 1.80                     | 0.64              |
| 49:BQ:108:GLY:HA3 | 58:BZ:116:VAL:HG11 | 1.80                     | 0.64              |
| 1:CA:633:G:H5'    | 1:CA:634:C:OP2     | 1.98                     | 0.64              |
| 4:CD:36:ARG:HH11  | 4:CD:36:ARG:CB     | 2.10                     | 0.64              |
| 5:CE:101:ILE:HD13 | 5:CE:118:ILE:O     | 1.98                     | 0.64              |
| 24:CY:226:ASN:C   | 24:CY:228:MET:H    | 2.02                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:CY:137:ASN:O    | 24:CY:262:SER:HA   | 1.97                     | 0.64              |
| 24:CY:289:ILE:HG22 | 24:CY:290:LYS:H    | 1.62                     | 0.64              |
| 24:CY:519:ARG:HD3  | 24:CY:676:TYR:O    | 1.98                     | 0.64              |
| 24:CY:90:PHE:HE2   | 61:CY:702:FUA:H9   | 1.62                     | 0.64              |
| 28:D3:59:VAL:HG12  | 28:D3:60:GLU:N     | 2.13                     | 0.64              |
| 35:DA:1036:G:OP1   | 42:DH:59:ARG:HD2   | 1.98                     | 0.64              |
| 35:DA:1943:U:H2'   | 35:DA:1943:U:O2    | 1.98                     | 0.64              |
| 35:DA:2442:C:H2'   | 35:DA:2443:C:H6    | 1.63                     | 0.64              |
| 35:DA:267:C:H2'    | 35:DA:268:C:H6     | 1.63                     | 0.64              |
| 35:DA:2735:G:H2'   | 35:DA:2736:G:H8    | 1.63                     | 0.64              |
| 35:DA:848:G:O6     | 35:DA:928:G:H2'    | 1.98                     | 0.64              |
| 40:DF:132:VAL:HG22 | 40:DF:133:ASN:H    | 1.62                     | 0.64              |
| 40:DF:32:LEU:C     | 40:DF:32:LEU:HD23  | 2.17                     | 0.64              |
| 46:DN:134:ARG:O    | 46:DN:136:GLU:N    | 2.31                     | 0.64              |
| 52:DT:83:ILE:HG13  | 52:DT:84:GLN:H     | 1.62                     | 0.64              |
| 57:DY:74:PRO:O     | 57:DY:80:GLY:HA2   | 1.97                     | 0.64              |
| 1:AA:1132:C:O2'    | 1:AA:1133:G:H5'    | 1.97                     | 0.64              |
| 4:AD:152:SER:O     | 4:AD:154:ASN:N     | 2.30                     | 0.64              |
| 6:AF:16:GLN:HA     | 6:AF:19:LEU:HB3    | 1.80                     | 0.64              |
| 10:AJ:23:ILE:HG22  | 10:AJ:23:ILE:O     | 1.98                     | 0.64              |
| 26:B1:41:ARG:HH22  | 35:BA:1365:A:H5'   | 1.61                     | 0.64              |
| 26:B1:90:ILE:HG22  | 26:B1:94:LEU:CD1   | 2.28                     | 0.64              |
| 26:B1:76:ARG:HH22  | 26:B1:95:LEU:HD22  | 1.63                     | 0.64              |
| 33:B8:32:LEU:HB3   | 33:B8:36:LYS:HZ2   | 1.63                     | 0.64              |
| 35:BA:1386:C:H2'   | 35:BA:1387:C:H6    | 1.63                     | 0.64              |
| 31:B6:37:ARG:HH22  | 35:BA:2286:A:H62   | 1.45                     | 0.64              |
| 41:BG:180:PHE:O    | 41:BG:182:LYS:N    | 2.31                     | 0.64              |
| 42:BH:156:ALA:O    | 42:BH:158:HIS:CD2  | 2.50                     | 0.64              |
| 42:BH:169:VAL:HG22 | 42:BH:170:ARG:N    | 2.12                     | 0.64              |
| 46:BN:55:VAL:HG21  | 46:BN:127:ASP:N    | 2.13                     | 0.64              |
| 50:BR:18:LEU:HD21  | 50:BR:22:ARG:NE    | 2.12                     | 0.64              |
| 53:BU:19:LYS:HB3   | 53:BU:20:LEU:HD22  | 1.80                     | 0.64              |
| 54:BV:38:LEU:HD23  | 54:BV:39:LEU:N     | 2.12                     | 0.64              |
| 1:CA:718:G:C8      | 11:CK:116:HIS:HB3  | 2.33                     | 0.64              |
| 1:CA:1348:U:H4'    | 9:CI:120:ARG:HG3   | 1.80                     | 0.64              |
| 10:CJ:34:VAL:CG2   | 10:CJ:74:ILE:HG22  | 2.24                     | 0.64              |
| 13:CM:27:LYS:HE2   | 13:CM:31:LYS:CE    | 2.23                     | 0.64              |
| 14:CN:29:ARG:HH11  | 14:CN:29:ARG:HG3   | 1.63                     | 0.64              |
| 16:CP:18:ARG:HD3   | 16:CP:35:LYS:HD2   | 1.80                     | 0.64              |
| 24:CY:117:GLN:HE22 | 24:CY:120:THR:HG23 | 1.63                     | 0.64              |
| 24:CY:678:GLU:HG2  | 24:CY:679:VAL:H    | 1.62                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 35:DA:1656:C:H2'    | 35:DA:1657:C:H6    | 1.61                     | 0.64              |
| 35:DA:654(R):C:HO2' | 35:DA:654(S):G:H8  | 1.45                     | 0.64              |
| 35:DA:965:C:H5'     | 35:DA:2273:A:C1'   | 2.23                     | 0.64              |
| 37:DC:57:GLN:HE21   | 37:DC:205:ALA:HA   | 1.63                     | 0.64              |
| 40:DF:123:LEU:HD13  | 40:DF:192:LEU:HD22 | 1.78                     | 0.64              |
| 44:DK:112:MET:HG3   | 44:DK:113:PRO:HD3  | 1.80                     | 0.64              |
| 47:DO:107:ARG:O     | 47:DO:112:MET:HE1  | 1.98                     | 0.64              |
| 49:DQ:87:LYS:HG2    | 49:DQ:88:GLY:H     | 1.60                     | 0.64              |
| 52:DT:1:MET:N       | 52:DT:7:ILE:HD11   | 2.13                     | 0.64              |
| 58:DZ:65:GLN:HB3    | 58:DZ:67:LEU:CD1   | 2.28                     | 0.64              |
| 22:AW:8:U:H3        | 22:AW:14:A:N6      | 1.95                     | 0.63              |
| 27:B2:63:VAL:HA     | 27:B2:66:GLU:HG2   | 1.80                     | 0.63              |
| 35:BA:1142(A):A:O2' | 35:BA:1143:A:H2'   | 1.98                     | 0.63              |
| 35:BA:1278:A:H5''   | 50:BR:36:THR:HG22  | 1.79                     | 0.63              |
| 35:BA:1435:G:H5'    | 35:BA:1436:G:OP2   | 1.97                     | 0.63              |
| 35:BA:2186:G:C2'    | 35:BA:2187:G:H5''  | 2.28                     | 0.63              |
| 35:BA:2639:A:H2'    | 35:BA:2640:G:O4'   | 1.97                     | 0.63              |
| 35:BA:35:G:O2'      | 35:BA:36:G:H5'     | 1.98                     | 0.63              |
| 38:BD:129:ASN:O     | 38:BD:193:VAL:HG12 | 1.98                     | 0.63              |
| 39:BE:117:MET:O     | 39:BE:117:MET:HG2  | 1.97                     | 0.63              |
| 41:BG:76:SER:CA     | 41:BG:83:ARG:HB3   | 2.28                     | 0.63              |
| 53:BU:83:LEU:HD12   | 53:BU:83:LEU:H     | 1.63                     | 0.63              |
| 55:BW:107:LEU:H     | 55:BW:107:LEU:HD22 | 1.63                     | 0.63              |
| 1:CA:163:C:O2'      | 1:CA:164:U:H5'     | 1.97                     | 0.63              |
| 1:CA:992:U:H1'      | 1:CA:993:G:C2      | 2.33                     | 0.63              |
| 4:CD:36:ARG:HH11    | 4:CD:36:ARG:HB3    | 1.61                     | 0.63              |
| 7:CG:7:ALA:O        | 7:CG:8:GLU:HB2     | 1.98                     | 0.63              |
| 22:CW:7:G:H3'       | 22:CW:8:U:C5'      | 2.28                     | 0.63              |
| 24:CY:512:ILE:H     | 24:CY:512:ILE:HD13 | 1.63                     | 0.63              |
| 25:D0:16:SER:HB2    | 35:DA:2262:U:C5    | 2.33                     | 0.63              |
| 35:DA:1775:U:H2'    | 35:DA:1776:G:C5'   | 2.28                     | 0.63              |
| 35:DA:2832:U:H1'    | 35:DA:2834:G:C2    | 2.33                     | 0.63              |
| 35:DA:392:C:H5''    | 35:DA:409:C:H5''   | 1.79                     | 0.63              |
| 35:DA:643:A:O2'     | 35:DA:644:A:H5'    | 1.97                     | 0.63              |
| 37:DC:213:VAL:HG12  | 37:DC:225:ILE:HD11 | 1.80                     | 0.63              |
| 38:DD:147:LEU:HD13  | 38:DD:155:LEU:CD1  | 2.26                     | 0.63              |
| 35:DA:1245:G:H5''   | 40:DF:34:TRP:HZ2   | 1.63                     | 0.63              |
| 49:DQ:24:GLY:O      | 49:DQ:102:VAL:HG23 | 1.98                     | 0.63              |
| 51:DS:59:LYS:HD2    | 51:DS:61:ASN:HB2   | 1.80                     | 0.63              |
| 51:DS:64:GLU:CD     | 51:DS:64:GLU:H     | 2.02                     | 0.63              |
| 49:DQ:137:TYR:OH    | 58:DZ:81:ARG:HD3   | 1.99                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:AA:1006:C:H2'     | 1:AA:1007:C:C6     | 2.32                     | 0.63              |
| 1:AA:301:G:O2'      | 1:AA:302:G:H5'     | 1.98                     | 0.63              |
| 1:AA:382:A:H2'      | 1:AA:383:A:H8      | 1.61                     | 0.63              |
| 1:AA:41:G:H2'       | 1:AA:42:G:H8       | 1.63                     | 0.63              |
| 1:AA:737:A:H2'      | 1:AA:738:C:C6      | 2.33                     | 0.63              |
| 4:AD:30:LYS:O       | 4:AD:32:ALA:N      | 2.31                     | 0.63              |
| 10:AJ:16:LEU:O      | 10:AJ:16:LEU:HD13  | 1.97                     | 0.63              |
| 1:AA:254:G:OP1      | 17:AQ:67:LYS:O     | 2.16                     | 0.63              |
| 26:B1:7:ILE:HG22    | 26:B1:8:SER:N      | 2.13                     | 0.63              |
| 26:B1:82:LEU:HD23   | 26:B1:90:ILE:HG23  | 1.81                     | 0.63              |
| 31:B6:19:ARG:O      | 31:B6:20:ASN:O     | 2.14                     | 0.63              |
| 35:BA:1064:C:H4'    | 44:BK:89:HIS:HD2   | 1.63                     | 0.63              |
| 35:BA:1831:G:H2'    | 35:BA:1832:C:C6    | 2.33                     | 0.63              |
| 35:BA:1948:G:H8     | 35:BA:1948:G:H5'   | 1.63                     | 0.63              |
| 38:BD:35:LYS:HG2    | 38:BD:63:ARG:CA    | 2.25                     | 0.63              |
| 39:BE:36:ARG:NH1    | 39:BE:36:ARG:HG2   | 2.12                     | 0.63              |
| 40:BF:78:ILE:HA     | 40:BF:83:PHE:CD1   | 2.32                     | 0.63              |
| 41:BG:10:LYS:HE2    | 41:BG:14:GLU:OE2   | 1.98                     | 0.63              |
| 47:BO:3:GLN:HB2     | 47:BO:4:PRO:HD2    | 1.81                     | 0.63              |
| 56:BX:41:ASN:C      | 56:BX:43:VAL:H     | 2.01                     | 0.63              |
| 1:CA:1281:U:H5''    | 1:CA:1282:C:H5     | 1.64                     | 0.63              |
| 1:CA:477:A:O2'      | 1:CA:479:C:H5'     | 1.97                     | 0.63              |
| 2:CB:140:HIS:O      | 2:CB:143:GLU:HB2   | 1.97                     | 0.63              |
| 24:CY:148:LEU:HD13  | 24:CY:151:ARG:HH11 | 1.63                     | 0.63              |
| 24:CY:193:GLY:HA3   | 24:CY:266:ASN:CB   | 2.27                     | 0.63              |
| 35:DA:1029:A:H5''   | 49:DQ:128:LYS:HE3  | 1.81                     | 0.63              |
| 35:DA:1747(A):G:O2' | 35:DA:1748:G:H5''  | 1.97                     | 0.63              |
| 35:DA:2018:G:H21    | 53:DU:34:LYS:NZ    | 1.96                     | 0.63              |
| 35:DA:240:G:C3'     | 35:DA:241:A:H5''   | 2.25                     | 0.63              |
| 35:DA:2795:G:H21    | 35:DA:2796:U:H5    | 1.47                     | 0.63              |
| 35:DA:365:C:C6      | 35:DA:365:C:H5'    | 2.33                     | 0.63              |
| 40:DF:160:ASN:HD21  | 40:DF:162:LEU:HB2  | 1.63                     | 0.63              |
| 42:DH:156:ALA:O     | 42:DH:158:HIS:N    | 2.31                     | 0.63              |
| 44:DK:17:ALA:HB3    | 44:DK:38:VAL:HG13  | 1.80                     | 0.63              |
| 54:DV:18:LEU:HD13   | 54:DV:19:LYS:H     | 1.61                     | 0.63              |
| 56:DX:12:VAL:CB     | 56:DX:17:ALA:HB1   | 2.11                     | 0.63              |
| 1:AA:129(A):G:H5''  | 1:AA:129(A):G:H8   | 1.63                     | 0.63              |
| 11:AK:59:TYR:CE2    | 11:AK:63:LEU:HD11  | 2.34                     | 0.63              |
| 26:B1:45:ASN:C      | 26:B1:45:ASN:ND2   | 2.49                     | 0.63              |
| 33:B8:50:LEU:HD12   | 33:B8:51:ALA:N     | 2.13                     | 0.63              |
| 35:BA:2008:C:H2'    | 35:BA:2009:G:H8    | 1.63                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:BA:203:C:C3'   | 35:BA:204:A:H5''   | 2.28                     | 0.63              |
| 35:BA:2396:G:O2'  | 35:BA:2397:G:H5'   | 1.99                     | 0.63              |
| 35:BA:2462:U:H2'  | 35:BA:2463:C:C6    | 2.34                     | 0.63              |
| 35:BA:26:G:H1'    | 35:BA:515:A:H61    | 1.64                     | 0.63              |
| 35:BA:322:A:OP2   | 40:BF:169:ASN:HB2  | 1.98                     | 0.63              |
| 40:BF:32:LEU:C    | 40:BF:32:LEU:HD23  | 2.18                     | 0.63              |
| 40:BF:38:ARG:O    | 40:BF:42:ALA:HB2   | 1.98                     | 0.63              |
| 41:BG:139:LEU:HA  | 41:BG:144:ILE:HG21 | 1.81                     | 0.63              |
| 41:BG:60:LEU:C    | 41:BG:63:ILE:HD11  | 2.17                     | 0.63              |
| 42:BH:149:ARG:HA  | 42:BH:162:ILE:CD1  | 2.29                     | 0.63              |
| 44:BK:112:MET:CE  | 44:BK:120:LEU:HD21 | 2.28                     | 0.63              |
| 46:BN:23:LEU:O    | 46:BN:23:LEU:HD23  | 1.97                     | 0.63              |
| 50:BR:100:LEU:N   | 50:BR:100:LEU:HD22 | 2.12                     | 0.63              |
| 53:BU:111:GLU:O   | 53:BU:115:ALA:HB2  | 1.98                     | 0.63              |
| 57:BY:95:LYS:HD3  | 57:BY:100:ALA:HB1  | 1.79                     | 0.63              |
| 6:CF:19:LEU:HD23  | 6:CF:19:LEU:O      | 1.97                     | 0.63              |
| 11:CK:85:ARG:HG2  | 11:CK:111:ASP:O    | 1.98                     | 0.63              |
| 11:CK:34:ASP:HB2  | 11:CK:35:PRO:CD    | 2.29                     | 0.63              |
| 19:CS:13:ASP:C    | 19:CS:15:LEU:H     | 2.01                     | 0.63              |
| 24:CY:15:ILE:O    | 24:CY:81:ILE:HA    | 1.99                     | 0.63              |
| 31:D6:15:GLU:CD   | 31:D6:44:ARG:NH1   | 2.52                     | 0.63              |
| 33:D8:50:LEU:C    | 33:D8:53:PRO:HD2   | 2.19                     | 0.63              |
| 35:DA:2131:G:H5'  | 35:DA:2133:G:H1'   | 1.80                     | 0.63              |
| 35:DA:2428:G:H5'  | 35:DA:2429:G:OP1   | 1.98                     | 0.63              |
| 35:DA:947:G:H2'   | 35:DA:948:G:H8     | 1.63                     | 0.63              |
| 27:D2:48:HIS:HD1  | 35:DA:95:G:HO2'    | 1.45                     | 0.63              |
| 38:DD:146:GLU:HG2 | 38:DD:152:GLY:C    | 2.19                     | 0.63              |
| 29:D4:7:PRO:CG    | 41:DG:61:ALA:HB1   | 2.29                     | 0.63              |
| 7:AG:27:ILE:CD1   | 7:AG:40:ALA:HA     | 2.28                     | 0.63              |
| 19:AS:13:ASP:C    | 19:AS:15:LEU:H     | 2.02                     | 0.63              |
| 22:AW:5:G:O2'     | 22:AW:6:G:H5'      | 1.99                     | 0.63              |
| 35:BA:2009:G:H1'  | 50:BR:107:ASP:O    | 1.98                     | 0.63              |
| 35:BA:2345:G:C5'  | 35:BA:2346:A:H5'   | 2.28                     | 0.63              |
| 35:BA:779:U:OP1   | 38:BD:49:ILE:HG23  | 1.98                     | 0.63              |
| 36:BB:40:U:O2     | 36:BB:43:C:H5''    | 1.99                     | 0.63              |
| 42:BH:153:LYS:HG3 | 42:BH:154:PRO:CD   | 2.28                     | 0.63              |
| 24:AY:662:LYS:NZ  | 42:BH:175:LYS:CD   | 2.61                     | 0.63              |
| 52:BT:27:THR:O    | 52:BT:28:VAL:CG2   | 2.46                     | 0.63              |
| 57:BY:88:LYS:NZ   | 57:BY:93:GLY:O     | 2.29                     | 0.63              |
| 1:CA:974:A:H8     | 1:CA:974:A:OP1     | 1.82                     | 0.63              |
| 12:CL:18:VAL:O    | 12:CL:19:ARG:HB3   | 1.98                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:CM:81:LEU:HD12  | 13:CM:86:CYS:SG    | 2.39                     | 0.63              |
| 24:CY:157:LEU:N    | 24:CY:157:LEU:HD23 | 2.09                     | 0.63              |
| 27:D2:16:LEU:CB    | 27:D2:20:GLU:HG2   | 2.26                     | 0.63              |
| 35:DA:1059:G:H2'   | 35:DA:1060:U:C6    | 2.33                     | 0.63              |
| 35:DA:2672:G:C2'   | 35:DA:2673:G:H5''  | 2.28                     | 0.63              |
| 37:DC:128:LEU:CD2  | 37:DC:132:LEU:CD1  | 2.75                     | 0.63              |
| 37:DC:176:VAL:HG21 | 37:DC:190:ILE:CD1  | 2.28                     | 0.63              |
| 39:DE:36:ARG:NH2   | 39:DE:88:GLY:H     | 1.97                     | 0.63              |
| 39:DE:98:PRO:HG3   | 39:DE:175:VAL:HG12 | 1.80                     | 0.63              |
| 35:DA:1061:U:O4    | 44:DK:52:ILE:HG21  | 1.99                     | 0.63              |
| 52:DT:30:VAL:HG21  | 52:DT:83:ILE:HG12  | 1.79                     | 0.63              |
| 35:DA:480:A:OP2    | 57:DY:46:LYS:HE2   | 1.99                     | 0.63              |
| 58:DZ:35:ARG:HG3   | 58:DZ:35:ARG:HH11  | 1.64                     | 0.63              |
| 1:AA:1003:G:C2     | 1:AA:1004:A:H1'    | 2.33                     | 0.63              |
| 1:AA:1281:U:H5''   | 1:AA:1282:C:H5     | 1.63                     | 0.63              |
| 1:AA:1435:G:H2'    | 1:AA:1436:U:C5     | 2.33                     | 0.63              |
| 1:AA:192:U:H2'     | 1:AA:193:C:C6      | 2.33                     | 0.63              |
| 2:AB:223:ILE:HA    | 2:AB:226:ARG:HB3   | 1.81                     | 0.63              |
| 12:AL:79:GLU:HB2   | 24:AY:442:THR:HG21 | 1.79                     | 0.63              |
| 24:AY:553:GLY:HA2  | 24:AY:560:VAL:CG2  | 2.28                     | 0.63              |
| 27:B2:69:ARG:CG    | 27:B2:70:GLN:N     | 2.59                     | 0.63              |
| 35:BA:1644:C:O2    | 35:BA:1644:C:H2'   | 1.98                     | 0.63              |
| 35:BA:2472:G:H3'   | 35:BA:2475:C:H42   | 1.64                     | 0.63              |
| 35:BA:55:G:H2'     | 35:BA:56:A:H8      | 1.63                     | 0.63              |
| 37:BC:99:GLU:O     | 37:BC:100:ILE:HD13 | 1.98                     | 0.63              |
| 37:BC:115:VAL:HA   | 37:BC:145:THR:HG22 | 1.80                     | 0.63              |
| 37:BC:71:LYS:HG2   | 37:BC:72:GLN:H     | 1.63                     | 0.63              |
| 48:BP:80:TYR:CD1   | 48:BP:111:ARG:HB3  | 2.34                     | 0.63              |
| 51:BS:98:VAL:HG12  | 51:BS:100:ALA:N    | 2.13                     | 0.63              |
| 58:BZ:153:SER:HB2  | 58:BZ:163:LEU:HD13 | 1.79                     | 0.63              |
| 1:CA:1269:A:C2     | 1:CA:1313:U:O4'    | 2.52                     | 0.63              |
| 1:CA:176:C:H2'     | 1:CA:177:C:C6      | 2.33                     | 0.63              |
| 1:CA:666:G:H5'     | 1:CA:726:C:H1'     | 1.80                     | 0.63              |
| 5:CE:64:ARG:HH11   | 5:CE:64:ARG:CG     | 2.09                     | 0.63              |
| 6:CF:33:TYR:HA     | 6:CF:71:ARG:NH2    | 2.11                     | 0.63              |
| 1:CA:191:G:N3      | 20:CT:105:SER:HB3  | 2.14                     | 0.63              |
| 20:CT:43:LEU:O     | 20:CT:46:GLU:N     | 2.32                     | 0.63              |
| 24:CY:652:MET:HA   | 24:CY:652:MET:CE   | 2.29                     | 0.63              |
| 28:D3:29:ARG:NH1   | 28:D3:29:ARG:HB2   | 2.14                     | 0.63              |
| 35:DA:1012:U:C4    | 46:DN:28:THR:HG21  | 2.33                     | 0.63              |
| 35:DA:2454:G:O2'   | 35:DA:2455:G:H5'   | 1.98                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:2855:C:H2'   | 35:DA:2856:C:H6    | 1.64                     | 0.63              |
| 35:DA:710:G:H2'    | 35:DA:711:G:H8     | 1.63                     | 0.63              |
| 35:DA:848:G:H5'    | 35:DA:849:A:OP2    | 1.98                     | 0.63              |
| 35:DA:958:U:H5'    | 49:DQ:14:ARG:HH11  | 1.62                     | 0.63              |
| 38:DD:161:THR:O    | 38:DD:196:VAL:HG23 | 1.98                     | 0.63              |
| 40:DF:38:ARG:O     | 40:DF:42:ALA:HB2   | 1.98                     | 0.63              |
| 41:DG:11:TYR:O     | 41:DG:15:VAL:HB    | 1.99                     | 0.63              |
| 47:DO:24:VAL:CG2   | 47:DO:30:ALA:HB3   | 2.27                     | 0.63              |
| 52:DT:33:LYS:HE2   | 52:DT:43:GLN:OE1   | 1.98                     | 0.63              |
| 53:DU:83:LEU:H     | 53:DU:83:LEU:HD12  | 1.64                     | 0.63              |
| 53:DU:88:ILE:O     | 53:DU:88:ILE:HG13  | 1.99                     | 0.63              |
| 1:AA:1403:C:O2     | 1:AA:1403:C:H2'    | 1.97                     | 0.63              |
| 4:AD:126:ILE:HG22  | 4:AD:127:THR:N     | 2.14                     | 0.63              |
| 4:AD:8:VAL:HB      | 4:AD:21:LEU:HD12   | 1.79                     | 0.63              |
| 6:AF:11:ASN:HB3    | 6:AF:14:LEU:HG     | 1.80                     | 0.63              |
| 16:AP:82:GLN:O     | 16:AP:84:ALA:N     | 2.31                     | 0.63              |
| 24:AY:227:ILE:HG22 | 24:AY:227:ILE:O    | 1.98                     | 0.63              |
| 24:AY:464:ASP:O    | 24:AY:468:ARG:HB2  | 1.99                     | 0.63              |
| 28:B3:52:HIS:CD2   | 28:B3:52:HIS:H     | 2.17                     | 0.63              |
| 30:B5:25:LEU:CD1   | 55:BW:19:LEU:HB3   | 2.28                     | 0.63              |
| 31:B6:11:LEU:HD22  | 31:B6:12:GLU:N     | 2.13                     | 0.63              |
| 33:B8:50:LEU:C     | 33:B8:53:PRO:HD2   | 2.19                     | 0.63              |
| 35:BA:2131:G:H5'   | 35:BA:2133:G:H1'   | 1.80                     | 0.63              |
| 35:BA:2248:C:H2'   | 35:BA:2249:U:H5'   | 1.81                     | 0.63              |
| 35:BA:252:G:OP2    | 48:BP:50:ARG:NH1   | 2.32                     | 0.63              |
| 35:BA:2720:U:H2'   | 35:BA:2721:A:C8    | 2.33                     | 0.63              |
| 38:BD:76:PRO:HG2   | 38:BD:98:VAL:HG21  | 1.81                     | 0.63              |
| 46:BN:46:VAL:O     | 46:BN:47:ALA:CB    | 2.46                     | 0.63              |
| 1:CA:1095:U:P      | 1:CA:1108:G:H1     | 2.21                     | 0.63              |
| 1:CA:559:A:H4'     | 1:CA:560:U:C5'     | 2.29                     | 0.63              |
| 3:CC:142:MET:CE    | 3:CC:171:GLY:HA3   | 2.28                     | 0.63              |
| 20:CT:42:GLN:HE21  | 20:CT:42:GLN:HA    | 1.64                     | 0.63              |
| 24:CY:276:VAL:O    | 24:CY:280:LEU:HD23 | 1.98                     | 0.63              |
| 35:DA:1510:G:O2'   | 35:DA:1511:C:H5'   | 1.99                     | 0.63              |
| 35:DA:2172:U:H1'   | 35:DA:2173:A:OP1   | 1.97                     | 0.63              |
| 35:DA:2348:U:C2'   | 35:DA:2349:G:H5''  | 2.28                     | 0.63              |
| 35:DA:2244:U:O2    | 35:DA:2434:A:H2'   | 1.98                     | 0.63              |
| 35:DA:311:A:H5'    | 35:DA:332:A:C2     | 2.33                     | 0.63              |
| 35:DA:790:C:H5'    | 35:DA:791:C:OP2    | 1.99                     | 0.63              |
| 48:DP:146:VAL:O    | 48:DP:148:LEU:N    | 2.32                     | 0.63              |
| 48:DP:16:ARG:CD    | 48:DP:18:ARG:H     | 2.08                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 56:DX:70:LEU:HD23 | 56:DX:71:GLY:N     | 2.14                     | 0.63              |
| 58:DZ:145:GLU:HG3 | 58:DZ:146:ILE:HG12 | 1.79                     | 0.63              |
| 1:AA:194:C:C2'    | 1:AA:195:A:H5''    | 2.29                     | 0.63              |
| 3:AC:181:ASN:HD22 | 3:AC:204:LEU:HB2   | 1.64                     | 0.63              |
| 9:AI:8:GLY:HA2    | 9:AI:79:LEU:HD12   | 1.81                     | 0.63              |
| 12:AL:75:HIS:HD2  | 12:AL:77:LEU:HD12  | 1.62                     | 0.63              |
| 13:AM:10:PRO:CB   | 13:AM:18:ALA:HB1   | 2.29                     | 0.63              |
| 24:AY:18:ALA:O    | 24:AY:19:ALA:HB2   | 1.99                     | 0.63              |
| 35:BA:221:A:H61   | 35:BA:265:A:H8     | 1.46                     | 0.63              |
| 35:BA:2259:G:O2'  | 35:BA:2260:C:H5'   | 1.99                     | 0.63              |
| 35:BA:2348:U:H2'  | 35:BA:2349:G:C5'   | 2.29                     | 0.63              |
| 35:BA:2762:G:H5'  | 35:BA:2762:G:C8    | 2.34                     | 0.63              |
| 35:BA:2876:G:H4'  | 52:BT:3:ARG:NE     | 2.12                     | 0.63              |
| 35:BA:491:G:H2'   | 35:BA:492:A:H8     | 1.62                     | 0.63              |
| 35:BA:629:G:H5''  | 35:BA:650:C:O2'    | 1.98                     | 0.63              |
| 35:BA:710:G:H2'   | 35:BA:711:G:H8     | 1.64                     | 0.63              |
| 38:BD:226:MET:HB3 | 38:BD:230:ASP:HB2  | 1.79                     | 0.63              |
| 38:BD:35:LYS:O    | 38:BD:36:PRO:C     | 2.37                     | 0.63              |
| 40:BF:167:ALA:HB1 | 40:BF:173:VAL:CG1  | 2.22                     | 0.63              |
| 1:CA:1002:G:H22   | 1:CA:1039:C:H2'    | 1.64                     | 0.63              |
| 1:CA:1492:A:H2'   | 1:CA:1493:A:C8     | 2.34                     | 0.63              |
| 1:CA:370:C:O2'    | 1:CA:371:G:H5'     | 1.98                     | 0.63              |
| 3:CC:113:ALA:HB3  | 3:CC:183:ASP:OD2   | 1.98                     | 0.63              |
| 3:CC:70:VAL:CG1   | 3:CC:71:ALA:H      | 2.07                     | 0.63              |
| 9:CI:114:TYR:HE1  | 10:CJ:60:ARG:N     | 1.95                     | 0.63              |
| 27:D2:69:ARG:O    | 27:D2:70:GLN:HB2   | 1.99                     | 0.63              |
| 33:D8:42:ARG:O    | 33:D8:44:LYS:N     | 2.29                     | 0.63              |
| 33:D8:56:GLU:HA   | 33:D8:59:LYS:HZ3   | 1.64                     | 0.63              |
| 35:DA:1237:A:O2'  | 35:DA:1238:G:O4'   | 2.16                     | 0.63              |
| 35:DA:769:G:O2'   | 35:DA:770:G:H5'    | 1.99                     | 0.63              |
| 35:DA:84:A:H5'    | 57:DY:9:LYS:HB3    | 1.81                     | 0.63              |
| 39:DE:8:LYS:O     | 39:DE:193:GLY:N    | 2.32                     | 0.63              |
| 50:DR:97:VAL:HG13 | 50:DR:114:VAL:HG22 | 1.79                     | 0.63              |
| 57:DY:51:VAL:HG12 | 57:DY:53:PRO:HD2   | 1.80                     | 0.63              |
| 1:AA:1128:C:H2'   | 1:AA:1129:C:C5'    | 2.24                     | 0.63              |
| 1:AA:512:U:H2'    | 1:AA:513:C:H6      | 1.64                     | 0.63              |
| 1:AA:824:C:H2'    | 1:AA:825:G:H8      | 1.64                     | 0.63              |
| 2:AB:111:ARG:HG2  | 2:AB:111:ARG:HH11  | 1.64                     | 0.63              |
| 2:AB:120:ALA:O    | 2:AB:121:LEU:HD23  | 1.99                     | 0.63              |
| 5:AE:72:GLN:HE22  | 5:AE:144:THR:HG22  | 1.62                     | 0.63              |
| 12:AL:27:LEU:HD21 | 12:AL:64:TYR:CE1   | 2.34                     | 0.63              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:390:C:O3'     | 16:AP:28:ARG:NH2  | 2.31                     | 0.63              |
| 22:AW:72:C:H2'     | 22:AW:73:A:C8     | 2.34                     | 0.63              |
| 35:BA:1835:G:H1'   | 35:BA:1931:U:O2   | 1.98                     | 0.63              |
| 31:B6:37:ARG:NH2   | 35:BA:2286:A:H62  | 1.96                     | 0.63              |
| 35:BA:2312:U:H4'   | 41:BG:71:THR:OG1  | 1.98                     | 0.63              |
| 35:BA:2344:U:O2'   | 35:BA:2345:G:H5'' | 1.98                     | 0.63              |
| 35:BA:2244:U:O2    | 35:BA:2434:A:H2'  | 1.98                     | 0.63              |
| 35:BA:286:C:H2'    | 35:BA:287:C:C6    | 2.34                     | 0.63              |
| 35:BA:603:A:H4'    | 35:BA:604:G:O5'   | 1.98                     | 0.63              |
| 27:B2:47:ASN:HB2   | 35:BA:95:G:H1'    | 1.80                     | 0.63              |
| 38:BD:72:LYS:HE2   | 38:BD:101:GLU:OE2 | 1.98                     | 0.63              |
| 51:BS:67:ARG:HB3   | 51:BS:71:ARG:HH22 | 1.63                     | 0.63              |
| 52:BT:42:ILE:O     | 52:BT:42:ILE:HG13 | 1.97                     | 0.63              |
| 57:BY:88:LYS:HZ3   | 57:BY:93:GLY:C    | 2.03                     | 0.63              |
| 57:BY:96:ILE:HD12  | 57:BY:99:CYS:SG   | 2.37                     | 0.63              |
| 1:CA:1305:G:OP1    | 21:CU:2:GLY:N     | 2.32                     | 0.63              |
| 1:CA:509:A:C5'     | 1:CA:510:A:OP2    | 2.34                     | 0.63              |
| 3:CC:110:ASN:OD1   | 3:CC:140:ARG:HD2  | 1.98                     | 0.63              |
| 4:CD:16:GLY:HA2    | 4:CD:33:MET:CE    | 2.28                     | 0.63              |
| 4:CD:108:LEU:HD21  | 4:CD:183:GLY:HA3  | 1.80                     | 0.63              |
| 16:CP:53:VAL:HG23  | 16:CP:54:GLU:N    | 2.13                     | 0.63              |
| 19:CS:24:ALA:O     | 19:CS:25:LYS:HB2  | 1.98                     | 0.63              |
| 20:CT:93:GLU:C     | 20:CT:95:ALA:H    | 2.01                     | 0.63              |
| 23:CX:16:A:H2'     | 23:CX:17:U:H6     | 1.63                     | 0.63              |
| 24:CY:530:VAL:HG12 | 24:CY:533:VAL:CG2 | 2.29                     | 0.63              |
| 25:D0:42:GLY:HA3   | 35:DA:2331:G:O4'  | 1.98                     | 0.63              |
| 28:D3:17:LYS:HZ3   | 28:D3:20:LYS:HE3  | 1.60                     | 0.63              |
| 35:DA:1141:U:H6    | 46:DN:63:THR:HG21 | 1.63                     | 0.63              |
| 35:DA:1717:G:C3'   | 35:DA:1718:G:H5'' | 2.29                     | 0.63              |
| 44:DK:58:THR:O     | 44:DK:66:THR:HG22 | 1.98                     | 0.63              |
| 47:DO:104:ARG:HH21 | 52:DT:33:LYS:CE   | 2.11                     | 0.63              |
| 50:DR:100:LEU:HD22 | 50:DR:100:LEU:N   | 2.11                     | 0.63              |
| 52:DT:35:LYS:NZ    | 52:DT:41:ARG:HH11 | 1.96                     | 0.63              |
| 56:DX:26:TYR:HD2   | 56:DX:92:LEU:HD12 | 1.63                     | 0.63              |
| 1:AA:1152:A:H5''   | 10:AJ:13:HIS:CD2  | 2.33                     | 0.63              |
| 1:AA:1510:U:O2     | 1:AA:1526:G:C2    | 2.52                     | 0.63              |
| 1:AA:1513:A:H2'    | 1:AA:1514:C:H6    | 1.62                     | 0.63              |
| 1:AA:191:G:N3      | 20:AT:105:SER:HB3 | 2.14                     | 0.63              |
| 10:AJ:71:LEU:HD12  | 10:AJ:72:VAL:N    | 2.13                     | 0.63              |
| 10:AJ:4:ILE:HB     | 10:AJ:74:ILE:CG1  | 2.29                     | 0.63              |
| 16:AP:53:VAL:HG23  | 16:AP:54:GLU:N    | 2.14                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 24:AY:316:ILE:HD12  | 24:AY:326:THR:HG22 | 1.80                     | 0.63              |
| 35:BA:1047:G:HO2'   | 35:BA:1110:G:H1    | 1.47                     | 0.63              |
| 35:BA:2131:G:H5'    | 35:BA:2133:G:C1'   | 2.29                     | 0.63              |
| 39:BE:101:ARG:HH11  | 39:BE:169:ASN:HD22 | 1.44                     | 0.63              |
| 35:BA:2052:G:H4'    | 39:BE:143:ASN:O    | 1.99                     | 0.63              |
| 39:BE:24:THR:HG22   | 39:BE:186:GLY:CA   | 2.27                     | 0.63              |
| 39:BE:69:LYS:H      | 39:BE:69:LYS:HE2   | 1.64                     | 0.63              |
| 41:BG:153:ARG:HB3   | 41:BG:153:ARG:NH1  | 2.14                     | 0.63              |
| 43:BJ:26:UNK:CA     | 43:BJ:84:UNK:HA    | 2.28                     | 0.63              |
| 35:BA:1030:G:OP2    | 49:BQ:128:LYS:HE2  | 1.98                     | 0.63              |
| 49:BQ:45:GLN:H      | 49:BQ:45:GLN:CD    | 2.00                     | 0.63              |
| 54:BV:79:VAL:O      | 54:BV:79:VAL:HG12  | 1.98                     | 0.63              |
| 58:BZ:120:ILE:O     | 58:BZ:120:ILE:HG22 | 1.99                     | 0.63              |
| 1:CA:512:U:H2'      | 1:CA:513:C:H6      | 1.63                     | 0.63              |
| 3:CC:181:ASN:HD22   | 3:CC:204:LEU:HB2   | 1.61                     | 0.63              |
| 19:CS:41:VAL:C      | 19:CS:43:GLU:H     | 2.02                     | 0.63              |
| 22:CW:31:G:O2'      | 22:CW:32:G:H5'     | 1.99                     | 0.63              |
| 24:CY:264:LEU:C     | 24:CY:264:LEU:HD23 | 2.19                     | 0.63              |
| 35:DA:2348:U:H2'    | 35:DA:2349:G:C5'   | 2.29                     | 0.63              |
| 35:DA:814:C:H2'     | 35:DA:815:C:H6     | 1.62                     | 0.63              |
| 36:DB:21:G:N3       | 36:DB:21:G:H2'     | 2.13                     | 0.63              |
| 38:DD:11:PRO:C      | 38:DD:13:ARG:H     | 2.02                     | 0.63              |
| 39:DE:8:LYS:HG2     | 39:DE:192:ASN:HA   | 1.81                     | 0.63              |
| 42:DH:156:ALA:O     | 42:DH:158:HIS:CD2  | 2.52                     | 0.63              |
| 46:DN:57:ALA:N      | 46:DN:124:ALA:HA   | 2.14                     | 0.63              |
| 46:DN:22:THR:HA     | 46:DN:61:ARG:O     | 1.99                     | 0.63              |
| 48:DP:97:PRO:O      | 48:DP:98:GLU:CB    | 2.46                     | 0.63              |
| 1:AA:384:G:H2'      | 1:AA:385:C:C6      | 2.34                     | 0.62              |
| 1:AA:579:G:C5'      | 1:AA:728:A:H1'     | 2.28                     | 0.62              |
| 22:AW:75:C:H2'      | 22:AW:76:C:O4'     | 1.99                     | 0.62              |
| 30:B5:40:LYS:HD3    | 30:B5:44:THR:HB    | 1.81                     | 0.62              |
| 31:B6:35:GLU:OE1    | 31:B6:35:GLU:HA    | 1.99                     | 0.62              |
| 35:BA:1127:A:H2'    | 35:BA:1128:A:H5''  | 1.80                     | 0.62              |
| 35:BA:1268:A:H2'    | 35:BA:1269:A:O4'   | 1.98                     | 0.62              |
| 35:BA:1747(A):G:O2' | 35:BA:1748:G:H5''  | 1.97                     | 0.62              |
| 36:BB:21:G:N3       | 36:BB:21:G:H2'     | 2.13                     | 0.62              |
| 40:BF:28:ILE:CD1    | 40:BF:28:ILE:H     | 2.12                     | 0.62              |
| 44:BK:56:GLU:O      | 44:BK:67:PHE:HA    | 1.99                     | 0.62              |
| 45:BL:15:UNK:CB     | 45:BM:11:UNK:HA    | 23.81                    | 0.62              |
| 35:BA:1012:U:H3     | 46:BN:25:ARG:HE    | 1.46                     | 0.62              |
| 52:BT:1:MET:N       | 52:BT:7:ILE:HD11   | 2.13                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:BU:88:ILE:HG13  | 53:BU:88:ILE:O     | 1.98                     | 0.62              |
| 1:CA:1026:G:C2'    | 1:CA:1027:C:H5'    | 2.29                     | 0.62              |
| 1:CA:160:A:H1'     | 1:CA:344:A:C8      | 2.34                     | 0.62              |
| 1:CA:203:U:H5''    | 1:CA:204:U:OP1     | 1.98                     | 0.62              |
| 31:D6:35:GLU:HB2   | 31:D6:51:GLU:HB2   | 1.80                     | 0.62              |
| 35:DA:1053:C:H3'   | 35:DA:1054:A:H5''  | 1.79                     | 0.62              |
| 35:DA:1748:G:H2'   | 35:DA:1749:A:O4'   | 1.99                     | 0.62              |
| 35:DA:2131:G:H5'   | 35:DA:2133:G:C1'   | 2.29                     | 0.62              |
| 35:DA:581:C:H2'    | 35:DA:582:G:H8     | 1.63                     | 0.62              |
| 38:DD:35:LYS:NZ    | 38:DD:36:PRO:HD3   | 2.02                     | 0.62              |
| 39:DE:47:VAL:HG23  | 39:DE:84:PHE:O     | 1.99                     | 0.62              |
| 41:DG:172:LEU:O    | 41:DG:172:LEU:HD23 | 1.99                     | 0.62              |
| 46:DN:96:GLU:H     | 46:DN:96:GLU:CD    | 2.01                     | 0.62              |
| 47:DO:69:ILE:N     | 47:DO:69:ILE:HD12  | 2.14                     | 0.62              |
| 48:DP:96:THR:O     | 48:DP:99:LEU:HB3   | 1.99                     | 0.62              |
| 49:DQ:56:ARG:NE    | 49:DQ:56:ARG:HA    | 2.14                     | 0.62              |
| 57:DY:97:ARG:HG3   | 57:DY:97:ARG:HH11  | 1.63                     | 0.62              |
| 58:DZ:79:ARG:O     | 58:DZ:80:ARG:HB2   | 1.99                     | 0.62              |
| 1:AA:1026:G:C2'    | 1:AA:1027:C:H5'    | 2.29                     | 0.62              |
| 1:AA:332:G:O2'     | 1:AA:333:G:H5'     | 1.99                     | 0.62              |
| 3:AC:114:PRO:HD3   | 3:AC:183:ASP:OD2   | 1.99                     | 0.62              |
| 7:AG:15:ASP:HB3    | 7:AG:20:ASP:H      | 1.64                     | 0.62              |
| 10:AJ:3:LYS:NZ     | 10:AJ:77:PRO:HD2   | 2.14                     | 0.62              |
| 12:AL:24:VAL:HG13  | 12:AL:98:TYR:CE2   | 2.34                     | 0.62              |
| 24:AY:165:GLN:HB2  | 24:AY:260:LEU:CD1  | 2.29                     | 0.62              |
| 24:AY:255:ILE:HG12 | 24:AY:256:THR:N    | 2.14                     | 0.62              |
| 24:AY:573:HIS:CD2  | 24:AY:576:ASP:H    | 2.15                     | 0.62              |
| 35:BA:1038:C:C3'   | 35:BA:1039:G:H5''  | 2.27                     | 0.62              |
| 35:BA:1059:G:H2'   | 35:BA:1060:U:C6    | 2.34                     | 0.62              |
| 35:BA:11:G:H22     | 35:BA:2628:C:P     | 2.22                     | 0.62              |
| 35:BA:1717:G:C3'   | 35:BA:1718:G:H5''  | 2.30                     | 0.62              |
| 35:BA:2795:G:H21   | 35:BA:2796:U:H5    | 1.46                     | 0.62              |
| 35:BA:840:C:C2'    | 35:BA:841:A:H5''   | 2.28                     | 0.62              |
| 38:BD:28:GLU:HB2   | 38:BD:29:PRO:CD    | 2.29                     | 0.62              |
| 42:BH:44:VAL:O     | 42:BH:50:VAL:HG13  | 1.99                     | 0.62              |
| 35:BA:1012:U:O4    | 46:BN:28:THR:HG21  | 1.98                     | 0.62              |
| 54:BV:32:THR:HG23  | 54:BV:59:ALA:O     | 2.00                     | 0.62              |
| 1:CA:1218:C:H2'    | 1:CA:1219:U:C6     | 2.35                     | 0.62              |
| 1:CA:1328:C:H2'    | 1:CA:1329:A:C8     | 2.34                     | 0.62              |
| 1:CA:1452:C:H1'    | 1:CA:1456:G:C2     | 2.33                     | 0.62              |
| 1:CA:383:A:H2'     | 1:CA:384:G:H5'     | 1.80                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:673:G:H2'     | 1:CA:674:G:C8      | 2.34                     | 0.62              |
| 2:CB:168:THR:CG2   | 2:CB:192:SER:HB3   | 2.23                     | 0.62              |
| 2:CB:21:ARG:HD2    | 2:CB:39:ILE:CG1    | 2.29                     | 0.62              |
| 16:CP:50:LYS:HG2   | 16:CP:51:VAL:N     | 2.13                     | 0.62              |
| 22:CV:1:C:H2'      | 22:CV:2:G:H8       | 1.64                     | 0.62              |
| 24:CY:601:ILE:C    | 24:CY:602:LEU:HD23 | 2.20                     | 0.62              |
| 33:D8:14:VAL:HG21  | 33:D8:22:VAL:HG13  | 1.80                     | 0.62              |
| 33:D8:47:LYS:NZ    | 33:D8:49:VAL:HG13  | 2.14                     | 0.62              |
| 35:DA:1120:G:H2'   | 35:DA:1121:C:C6    | 2.34                     | 0.62              |
| 35:DA:1523:U:H2'   | 35:DA:1524:G:C8    | 2.33                     | 0.62              |
| 35:DA:2552:U:C2    | 35:DA:2554:U:H5'   | 2.34                     | 0.62              |
| 37:DC:65:LEU:HD13  | 37:DC:189:ASN:ND2  | 2.14                     | 0.62              |
| 38:DD:28:GLU:HB2   | 38:DD:29:PRO:CD    | 2.29                     | 0.62              |
| 41:DG:55:LYS:HG2   | 41:DG:58:GLN:HE21  | 1.63                     | 0.62              |
| 49:DQ:60:ARG:HB2   | 49:DQ:60:ARG:NH1   | 2.14                     | 0.62              |
| 50:DR:78:LYS:O     | 50:DR:83:ILE:HG12  | 1.99                     | 0.62              |
| 54:DV:79:VAL:O     | 54:DV:79:VAL:HG12  | 1.99                     | 0.62              |
| 58:DZ:180:VAL:O    | 58:DZ:182:LYS:N    | 2.32                     | 0.62              |
| 1:AA:1054:C:OP2    | 1:AA:1197:G:OP2    | 2.17                     | 0.62              |
| 1:AA:1250:A:H2'    | 1:AA:1251:A:C8     | 2.34                     | 0.62              |
| 4:AD:18:LYS:C      | 4:AD:19:LEU:HD12   | 2.20                     | 0.62              |
| 4:AD:57:ARG:HB3    | 4:AD:206:PHE:HB2   | 1.81                     | 0.62              |
| 15:AO:83:GLU:C     | 15:AO:85:LEU:H     | 2.02                     | 0.62              |
| 22:AW:50:G:H2'     | 22:AW:51:U:O4'     | 1.99                     | 0.62              |
| 28:B3:4:LEU:HD11   | 28:B3:39:ASP:OD1   | 1.99                     | 0.62              |
| 31:B6:5:VAL:HG12   | 31:B6:6:ARG:N      | 2.14                     | 0.62              |
| 33:B8:51:ALA:C     | 33:B8:53:PRO:HD2   | 2.19                     | 0.62              |
| 39:BE:47:VAL:HG23  | 39:BE:84:PHE:O     | 1.98                     | 0.62              |
| 35:BA:2631:G:N2    | 39:BE:61:ARG:NH1   | 2.47                     | 0.62              |
| 39:BE:36:ARG:NH2   | 39:BE:88:GLY:H     | 1.97                     | 0.62              |
| 42:BH:124:GLU:HG3  | 42:BH:132:ARG:HG3  | 1.80                     | 0.62              |
| 35:BA:1061:U:O4    | 44:BK:52:ILE:HG21  | 1.99                     | 0.62              |
| 44:BK:79:ARG:HD2   | 44:BK:85:GLU:O     | 1.99                     | 0.62              |
| 50:BR:28:LEU:HD23  | 50:BR:28:LEU:C     | 2.20                     | 0.62              |
| 51:BS:97:ARG:HE    | 51:BS:97:ARG:C     | 2.03                     | 0.62              |
| 52:BT:132:LYS:CD   | 52:BT:132:LYS:H    | 2.11                     | 0.62              |
| 57:BY:62:GLU:CG    | 57:BY:63:LYS:H     | 2.11                     | 0.62              |
| 58:BZ:105:VAL:HG13 | 58:BZ:105:VAL:O    | 1.99                     | 0.62              |
| 58:BZ:42:VAL:HG13  | 58:BZ:43:GLU:N     | 2.14                     | 0.62              |
| 1:CA:781:A:H4'     | 1:CA:1522:U:O2'    | 1.98                     | 0.62              |
| 4:CD:173:TRP:HB3   | 4:CD:187:ARG:NH1   | 2.14                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:CF:71:ARG:HH11   | 6:CF:71:ARG:HG3    | 1.62                     | 0.62              |
| 7:CG:15:ASP:HB3    | 7:CG:20:ASP:H      | 1.64                     | 0.62              |
| 22:CW:52:C:C3'     | 22:CW:53:G:H5''    | 2.29                     | 0.62              |
| 24:CY:259:PHE:C    | 24:CY:260:LEU:HD13 | 2.19                     | 0.62              |
| 24:CY:293:THR:C    | 24:CY:295:GLU:H    | 2.02                     | 0.62              |
| 24:CY:90:PHE:CZ    | 61:CY:702:FUA:H121 | 2.34                     | 0.62              |
| 35:DA:1329:U:H5'   | 35:DA:1330:C:H5    | 1.63                     | 0.62              |
| 35:DA:1380:G:H2'   | 35:DA:1381:G:H8    | 1.64                     | 0.62              |
| 35:DA:1717:G:H2'   | 35:DA:1718:G:H5''  | 1.80                     | 0.62              |
| 35:DA:2248:C:H2'   | 35:DA:2249:U:H5'   | 1.80                     | 0.62              |
| 25:D0:16:SER:OG    | 35:DA:2261:C:H3'   | 1.99                     | 0.62              |
| 35:DA:2262:U:O2'   | 35:DA:2263:C:H5''  | 1.98                     | 0.62              |
| 50:DR:97:VAL:HA    | 50:DR:113:LEU:O    | 2.00                     | 0.62              |
| 52:DT:106:SER:O    | 52:DT:107:ASP:HB3  | 1.97                     | 0.62              |
| 1:AA:793:U:H3'     | 1:AA:794:A:C5'     | 2.22                     | 0.62              |
| 1:AA:8:A:N6        | 4:AD:209:ARG:HB2   | 2.12                     | 0.62              |
| 8:AH:104:ARG:O     | 8:AH:106:GLY:N     | 2.33                     | 0.62              |
| 1:AA:692:U:OP1     | 11:AK:124:LYS:HE2  | 1.99                     | 0.62              |
| 13:AM:97:PRO:CA    | 13:AM:110:ARG:HD3  | 2.26                     | 0.62              |
| 17:AQ:66:SER:O     | 17:AQ:70:ARG:NH1   | 2.33                     | 0.62              |
| 18:AR:45:SER:H     | 18:AR:51:LEU:HG    | 1.62                     | 0.62              |
| 24:AY:201:ILE:N    | 24:AY:201:ILE:HD12 | 2.13                     | 0.62              |
| 26:B1:57:GLU:HG2   | 26:B1:58:ILE:H     | 1.64                     | 0.62              |
| 26:B1:86:SER:HB2   | 26:B1:90:ILE:HD11  | 1.80                     | 0.62              |
| 31:B6:11:LEU:HG    | 31:B6:26:ASN:ND2   | 2.13                     | 0.62              |
| 33:B8:42:ARG:O     | 33:B8:44:LYS:N     | 2.29                     | 0.62              |
| 35:BA:2228:G:H2'   | 35:BA:2229:C:C6    | 2.34                     | 0.62              |
| 35:BA:2262:U:O2'   | 35:BA:2263:C:H5''  | 1.99                     | 0.62              |
| 37:BC:73:VAL:HG11  | 37:BC:158:LYS:HA   | 1.81                     | 0.62              |
| 39:BE:101:ARG:HH11 | 39:BE:169:ASN:ND2  | 1.98                     | 0.62              |
| 40:BF:123:LEU:CD1  | 40:BF:192:LEU:HD22 | 2.29                     | 0.62              |
| 41:BG:16:ARG:NE    | 41:BG:31:VAL:HG11  | 2.14                     | 0.62              |
| 48:BP:97:PRO:O     | 48:BP:98:GLU:CB    | 2.46                     | 0.62              |
| 50:BR:117:VAL:HG12 | 50:BR:118:GLU:N    | 2.13                     | 0.62              |
| 55:BW:88:ARG:HB3   | 55:BW:92:ARG:HB3   | 1.81                     | 0.62              |
| 1:CA:1137:C:H4'    | 1:CA:1138:G:C2     | 2.34                     | 0.62              |
| 1:CA:1346:A:N1     | 1:CA:1374:A:H5''   | 2.14                     | 0.62              |
| 1:CA:384:G:H2'     | 1:CA:385:C:C6      | 2.34                     | 0.62              |
| 1:CA:692:U:OP1     | 11:CK:124:LYS:HE2  | 2.00                     | 0.62              |
| 1:CA:740:U:O2'     | 1:CA:741:G:H5'     | 1.99                     | 0.62              |
| 1:CA:955:U:O2'     | 1:CA:956:U:H5'     | 1.99                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:CC:11:ARG:O      | 3:CC:13:GLY:N      | 2.33                     | 0.62              |
| 4:CD:13:ARG:HA     | 4:CD:33:MET:HE1    | 1.81                     | 0.62              |
| 21:CU:6:ARG:HH21   | 21:CU:15:ARG:NH2   | 1.97                     | 0.62              |
| 24:CY:242:LEU:O    | 24:CY:245:ALA:HB3  | 1.99                     | 0.62              |
| 35:DA:1332:G:H22   | 35:DA:1609:A:H3'   | 1.64                     | 0.62              |
| 35:DA:1917:U:C2'   | 35:DA:1918:A:H5'   | 2.28                     | 0.62              |
| 35:DA:2345:G:O2'   | 35:DA:2381:C:H2'   | 2.00                     | 0.62              |
| 36:DB:54:G:O2'     | 36:DB:55:U:H5'     | 1.99                     | 0.62              |
| 40:DF:53:THR:CG2   | 40:DF:56:GLU:HG3   | 2.21                     | 0.62              |
| 52:DT:38:ASN:ND2   | 52:DT:40:THR:H     | 1.98                     | 0.62              |
| 58:DZ:37:VAL:HG23  | 58:DZ:38:TYR:N     | 2.13                     | 0.62              |
| 1:AA:1049:U:H1'    | 1:AA:1201:A:N7     | 2.13                     | 0.62              |
| 1:AA:1334:G:H5'    | 1:AA:1335:C:OP2    | 1.99                     | 0.62              |
| 1:AA:662:G:H2'     | 1:AA:663:A:H8      | 1.64                     | 0.62              |
| 2:AB:14:GLY:O      | 2:AB:15:VAL:HG13   | 2.00                     | 0.62              |
| 2:AB:172:ILE:HD12  | 2:AB:172:ILE:N     | 2.13                     | 0.62              |
| 4:AD:173:TRP:HB3   | 4:AD:187:ARG:NH1   | 2.15                     | 0.62              |
| 7:AG:102:ARG:HG2   | 7:AG:106:GLN:NE2   | 2.13                     | 0.62              |
| 18:AR:40:LEU:O     | 18:AR:42:ARG:N     | 2.33                     | 0.62              |
| 24:AY:165:GLN:C    | 24:AY:166:LEU:HD12 | 2.20                     | 0.62              |
| 24:AY:662:LYS:NZ   | 42:BH:175:LYS:CG   | 2.63                     | 0.62              |
| 35:BA:2428:G:H5'   | 35:BA:2429:G:OP1   | 2.00                     | 0.62              |
| 35:BA:2672:G:C2'   | 35:BA:2673:G:H5''  | 2.29                     | 0.62              |
| 35:BA:2735:G:H2'   | 35:BA:2736:G:H8    | 1.63                     | 0.62              |
| 35:BA:581:C:H2'    | 35:BA:582:G:H8     | 1.62                     | 0.62              |
| 35:BA:589:C:O2'    | 35:BA:590:A:H5'    | 1.99                     | 0.62              |
| 25:B0:26:TYR:HE2   | 35:BA:857:C:H1'    | 1.65                     | 0.62              |
| 35:BA:947:G:H2'    | 35:BA:948:G:H8     | 1.64                     | 0.62              |
| 38:BD:158:ALA:HB3  | 38:BD:161:THR:CG2  | 2.29                     | 0.62              |
| 42:BH:136:ILE:HD12 | 42:BH:136:ILE:N    | 2.14                     | 0.62              |
| 44:BK:41:PHE:CE1   | 44:BK:45:THR:HG21  | 2.34                     | 0.62              |
| 50:BR:97:VAL:HG13  | 50:BR:114:VAL:HG22 | 1.81                     | 0.62              |
| 52:BT:10:VAL:O     | 52:BT:12:SER:N     | 2.33                     | 0.62              |
| 53:BU:80:ILE:O     | 53:BU:84:LYS:HB2   | 2.00                     | 0.62              |
| 58:BZ:59:LEU:HD11  | 58:BZ:88:PHE:CD2   | 2.35                     | 0.62              |
| 1:CA:1003:G:C2     | 1:CA:1004:A:H1'    | 2.35                     | 0.62              |
| 1:CA:579:G:C5'     | 1:CA:728:A:H1'     | 2.28                     | 0.62              |
| 2:CB:120:ALA:O     | 2:CB:121:LEU:HD23  | 2.00                     | 0.62              |
| 2:CB:223:ILE:HA    | 2:CB:226:ARG:HB3   | 1.81                     | 0.62              |
| 2:CB:220:ASP:O     | 2:CB:223:ILE:HG13  | 1.99                     | 0.62              |
| 4:CD:121:VAL:HA    | 4:CD:126:ILE:HD13  | 1.81                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:CJ:23:ILE:HG22  | 10:CJ:23:ILE:O     | 1.99                     | 0.62              |
| 10:CJ:30:SER:OG    | 10:CJ:81:THR:HG22  | 1.99                     | 0.62              |
| 10:CJ:32:ALA:HB1   | 10:CJ:75:ILE:HG13  | 1.81                     | 0.62              |
| 10:CJ:75:ILE:CG1   | 10:CJ:76:ASN:H     | 2.04                     | 0.62              |
| 24:CY:541:ALA:HB2  | 24:CY:579:GLU:HG2  | 1.81                     | 0.62              |
| 28:D3:36:VAL:O     | 28:D3:37:LEU:HD23  | 2.00                     | 0.62              |
| 19:CS:9:VAL:HG23   | 29:D4:53:GLU:OE2   | 1.99                     | 0.62              |
| 35:DA:139(A):G:H22 | 56:DX:44:GLU:CD    | 2.03                     | 0.62              |
| 35:DA:1504:C:C2'   | 35:DA:1505:C:H5''  | 2.30                     | 0.62              |
| 35:DA:2298:A:H62   | 35:DA:2318:G:H8    | 1.47                     | 0.62              |
| 35:DA:2555:U:H2'   | 35:DA:2556:C:H5'   | 1.80                     | 0.62              |
| 35:DA:2639:A:H2'   | 35:DA:2640:G:O4'   | 1.99                     | 0.62              |
| 35:DA:310:A:OP2    | 57:DY:18:GLY:HA2   | 1.99                     | 0.62              |
| 35:DA:840:C:C2'    | 35:DA:841:A:H5''   | 2.29                     | 0.62              |
| 39:DE:59:VAL:HG22  | 39:DE:62:PRO:O     | 1.99                     | 0.62              |
| 42:DH:19:VAL:HG12  | 42:DH:20:ALA:N     | 2.13                     | 0.62              |
| 46:DN:67:LEU:CD2   | 46:DN:87:LEU:HB3   | 2.30                     | 0.62              |
| 51:DS:67:ARG:HB3   | 51:DS:71:ARG:NH2   | 2.14                     | 0.62              |
| 54:DV:38:LEU:HD23  | 54:DV:39:LEU:N     | 2.14                     | 0.62              |
| 58:DZ:153:SER:C    | 58:DZ:155:LEU:HD23 | 2.20                     | 0.62              |
| 1:AA:291:C:O2'     | 1:AA:292:G:H5'     | 1.99                     | 0.62              |
| 1:AA:633:G:H5'     | 1:AA:634:C:OP2     | 1.99                     | 0.62              |
| 3:AC:113:ALA:HB3   | 3:AC:183:ASP:OD2   | 1.98                     | 0.62              |
| 4:AD:16:GLY:HA2    | 4:AD:33:MET:HE1    | 1.82                     | 0.62              |
| 1:AA:1250:A:H4'    | 9:AI:68:GLY:N      | 2.14                     | 0.62              |
| 12:AL:23:LYS:O     | 12:AL:24:VAL:HG23  | 2.00                     | 0.62              |
| 18:AR:37:VAL:CG2   | 18:AR:38:GLU:H     | 2.08                     | 0.62              |
| 20:AT:43:LEU:HB3   | 20:AT:48:LYS:HB2   | 1.82                     | 0.62              |
| 22:AV:47:U:H3'     | 22:AV:48:C:H5'     | 1.82                     | 0.62              |
| 28:B3:29:ARG:NH1   | 28:B3:29:ARG:HB2   | 2.14                     | 0.62              |
| 33:B8:25:MET:HG3   | 48:BP:64:LYS:HB2   | 1.82                     | 0.62              |
| 35:BA:1441:G:H2'   | 35:BA:1442:G:H8    | 1.65                     | 0.62              |
| 26:B1:47:GLN:HG3   | 35:BA:2091:U:O2'   | 2.00                     | 0.62              |
| 35:BA:2168:G:N2    | 35:BA:2170:A:H3'   | 2.14                     | 0.62              |
| 35:BA:2199:A:H3'   | 35:BA:2200:C:H6    | 1.65                     | 0.62              |
| 35:BA:2344:U:H4'   | 35:BA:2345:G:OP1   | 1.98                     | 0.62              |
| 35:BA:94:C:H5'     | 35:BA:94(A):G:OP2  | 2.00                     | 0.62              |
| 42:BH:98:LEU:HD12  | 42:BH:102:ALA:O    | 1.99                     | 0.62              |
| 48:BP:41:ARG:HA    | 48:BP:41:ARG:NH2   | 2.07                     | 0.62              |
| 51:BS:106:ARG:HB3  | 51:BS:106:ARG:NH1  | 2.13                     | 0.62              |
| 52:BT:25:GLY:HA2   | 52:BT:92:GLY:CA    | 2.29                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:BX:26:TYR:HD2   | 56:BX:92:LEU:HD12  | 1.65                     | 0.62              |
| 1:CA:250:A:H4'     | 1:CA:251:G:O5'     | 1.99                     | 0.62              |
| 2:CB:215:LEU:O     | 2:CB:219:VAL:HG23  | 2.00                     | 0.62              |
| 3:CC:114:PRO:HD3   | 3:CC:183:ASP:OD2   | 1.99                     | 0.62              |
| 4:CD:8:VAL:HB      | 4:CD:21:LEU:HD12   | 1.82                     | 0.62              |
| 6:CF:69:GLU:O      | 6:CF:72:VAL:HG12   | 2.00                     | 0.62              |
| 1:CA:1148:U:O3'    | 9:CI:14:VAL:HG11   | 2.00                     | 0.62              |
| 20:CT:29:LYS:O     | 20:CT:33:ILE:HG13  | 2.00                     | 0.62              |
| 20:CT:33:ILE:HD13  | 20:CT:63:ILE:HG12  | 1.81                     | 0.62              |
| 23:CX:12:A:H2      | 23:CX:13:A:H5'     | 1.64                     | 0.62              |
| 24:CY:243:VAL:HG13 | 24:CY:279:TYR:CE1  | 2.35                     | 0.62              |
| 24:CY:630:GLN:HE22 | 24:CY:646:PHE:HD2  | 1.46                     | 0.62              |
| 35:DA:570:G:H2'    | 35:DA:2030:A:N7    | 2.14                     | 0.62              |
| 35:DA:336:C:H4'    | 57:DY:7:VAL:HG21   | 1.80                     | 0.62              |
| 35:DA:52:A:O2'     | 35:DA:53:A:H5'     | 1.99                     | 0.62              |
| 35:DA:748:G:O6     | 35:DA:751:A:H4'    | 1.98                     | 0.62              |
| 37:DC:115:VAL:HG12 | 37:DC:145:THR:HG23 | 1.81                     | 0.62              |
| 38:DD:72:LYS:HE2   | 38:DD:101:GLU:OE2  | 1.99                     | 0.62              |
| 41:DG:77:ILE:CG2   | 41:DG:80:PHE:HB2   | 2.29                     | 0.62              |
| 46:DN:45:ASN:H     | 46:DN:45:ASN:ND2   | 1.93                     | 0.62              |
| 48:DP:23:PRO:O     | 48:DP:33:ARG:HD2   | 2.00                     | 0.62              |
| 48:DP:96:THR:HG22  | 48:DP:126:VAL:HB   | 1.81                     | 0.62              |
| 1:AA:250:A:H4'     | 1:AA:251:G:O5'     | 1.99                     | 0.62              |
| 1:AA:718:G:C8      | 11:AK:116:HIS:HB3  | 2.34                     | 0.62              |
| 2:AB:80:ILE:H      | 2:AB:80:ILE:HD12   | 1.63                     | 0.62              |
| 8:AH:5:PRO:O       | 8:AH:8:ASP:HB3     | 1.99                     | 0.62              |
| 24:AY:111:SER:O    | 24:AY:113:GLY:N    | 2.33                     | 0.62              |
| 24:AY:17:ILE:N     | 24:AY:17:ILE:HD12  | 2.14                     | 0.62              |
| 25:B0:27:GLU:N     | 25:B0:27:GLU:CD    | 2.41                     | 0.62              |
| 30:B5:56:LYS:HG3   | 30:B5:57:VAL:N     | 2.11                     | 0.62              |
| 31:B6:45:LYS:HG2   | 35:BA:2371:G:H4'   | 1.80                     | 0.62              |
| 31:B6:6:ARG:HD2    | 31:B6:6:ARG:H      | 1.64                     | 0.62              |
| 35:BA:965:C:C4'    | 35:BA:2273:A:H1'   | 2.29                     | 0.62              |
| 42:BH:30:LYS:CD    | 42:BH:81:GLU:HG2   | 2.29                     | 0.62              |
| 51:BS:40:ILE:HG22  | 51:BS:41:ASP:N     | 2.14                     | 0.62              |
| 52:BT:106:SER:O    | 52:BT:107:ASP:HB3  | 2.00                     | 0.62              |
| 54:BV:47:VAL:HB    | 54:BV:50:PRO:O     | 1.99                     | 0.62              |
| 1:CA:1284:C:H3'    | 1:CA:1285:A:C5'    | 2.28                     | 0.62              |
| 2:CB:156:LYS:O     | 2:CB:157:ARG:HB3   | 1.98                     | 0.62              |
| 3:CC:150:LYS:HB2   | 3:CC:169:ALA:HB2   | 1.80                     | 0.62              |
| 5:CE:51:VAL:O      | 5:CE:55:VAL:HG23   | 2.00                     | 0.62              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:CF:16:GLN:HA     | 6:CF:19:LEU:HB3    | 1.81                     | 0.62              |
| 1:CA:1152:A:H5''   | 10:CJ:13:HIS:CD2   | 2.34                     | 0.62              |
| 13:CM:15:VAL:HG12  | 13:CM:45:VAL:CG2   | 2.28                     | 0.62              |
| 20:CT:45:GLN:HA    | 20:CT:91:LEU:HB3   | 1.82                     | 0.62              |
| 24:CY:128:TYR:CE2  | 24:CY:130:VAL:HG23 | 2.33                     | 0.62              |
| 24:CY:289:ILE:CG2  | 24:CY:290:LYS:H    | 2.12                     | 0.62              |
| 24:CY:512:ILE:HG22 | 24:CY:567:LEU:HA   | 1.81                     | 0.62              |
| 24:CY:646:PHE:O    | 24:CY:647:VAL:HG13 | 1.99                     | 0.62              |
| 24:CY:688:ILE:O    | 24:CY:688:ILE:HG22 | 1.98                     | 0.62              |
| 30:D5:40:LYS:HE2   | 30:D5:46:CYS:HB3   | 1.81                     | 0.62              |
| 33:D8:32:LEU:HB3   | 33:D8:36:LYS:HZ2   | 1.65                     | 0.62              |
| 35:DA:272(B):G:H2' | 35:DA:272(C):G:C8  | 2.34                     | 0.62              |
| 35:DA:896:A:O4'    | 58:DZ:146:ILE:HD12 | 2.00                     | 0.62              |
| 38:DD:186:HIS:HD2  | 38:DD:188:GLU:H    | 1.46                     | 0.62              |
| 39:DE:48:GLN:HE21  | 39:DE:78:LEU:HD22  | 1.64                     | 0.62              |
| 52:DT:132:LYS:CD   | 52:DT:132:LYS:H    | 2.13                     | 0.62              |
| 58:DZ:55:HIS:O     | 58:DZ:57:ILE:HD12  | 2.00                     | 0.62              |
| 10:AJ:32:ALA:HB1   | 10:AJ:75:ILE:HG13  | 1.82                     | 0.62              |
| 13:AM:81:LEU:HD12  | 13:AM:86:CYS:SG    | 2.39                     | 0.62              |
| 22:AV:47:U:H3'     | 22:AV:48:C:C5'     | 2.30                     | 0.62              |
| 24:AY:9:LEU:C      | 24:AY:11:ARG:H     | 2.03                     | 0.62              |
| 35:BA:1223:G:H5'   | 35:BA:1224:C:OP2   | 1.98                     | 0.62              |
| 35:BA:1541:G:O2'   | 35:BA:1542:A:H5''  | 1.99                     | 0.62              |
| 35:BA:1842:G:H2'   | 35:BA:1843:C:C6    | 2.34                     | 0.62              |
| 35:BA:1946:U:H2'   | 35:BA:1947:C:H6    | 1.64                     | 0.62              |
| 38:BD:232:PRO:HD2  | 38:BD:249:PRO:HA   | 1.82                     | 0.62              |
| 39:BE:59:VAL:HG22  | 39:BE:62:PRO:O     | 2.00                     | 0.62              |
| 41:BG:77:ILE:HG21  | 41:BG:80:PHE:HB2   | 1.79                     | 0.62              |
| 1:CA:1303:C:H2'    | 1:CA:1304:G:H5'    | 1.81                     | 0.62              |
| 1:CA:72:C:H2'      | 1:CA:73:G:H8       | 1.64                     | 0.62              |
| 12:CL:18:VAL:HG23  | 12:CL:19:ARG:N     | 2.07                     | 0.62              |
| 13:CM:4:ILE:HG22   | 13:CM:5:ALA:H      | 1.64                     | 0.62              |
| 16:CP:82:GLN:O     | 16:CP:84:ALA:N     | 2.32                     | 0.62              |
| 20:CT:13:LEU:HD12  | 20:CT:13:LEU:N     | 2.13                     | 0.62              |
| 24:CY:289:ILE:CG2  | 24:CY:290:LYS:N    | 2.62                     | 0.62              |
| 35:DA:2720:U:H2'   | 35:DA:2721:A:C8    | 2.34                     | 0.62              |
| 35:DA:363(D):G:O2' | 35:DA:363(E):U:H5' | 2.00                     | 0.62              |
| 35:DA:94:C:H5'     | 35:DA:94(A):G:OP2  | 1.99                     | 0.62              |
| 39:DE:69:LYS:H     | 39:DE:69:LYS:HE2   | 1.64                     | 0.62              |
| 44:DK:112:MET:CE   | 44:DK:120:LEU:HD21 | 2.30                     | 0.62              |
| 45:DL:62:UNK:HA    | 45:DL:120:UNK:CB   | 2.29                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 54:DV:18:LEU:HD13  | 54:DV:19:LYS:N     | 2.15                     | 0.62              |
| 54:DV:32:THR:HG1   | 54:DV:60:GLU:HG3   | 1.65                     | 0.62              |
| 55:DW:88:ARG:HB3   | 55:DW:92:ARG:HB3   | 1.82                     | 0.62              |
| 1:AA:1415:G:H2'    | 1:AA:1416:G:H8     | 1.65                     | 0.62              |
| 1:AA:203:U:H5''    | 1:AA:204:U:OP1     | 2.00                     | 0.62              |
| 1:AA:383:A:H2'     | 1:AA:384:G:H5'     | 1.82                     | 0.62              |
| 24:AY:162:VAL:O    | 24:AY:164:MET:HG2  | 1.98                     | 0.62              |
| 24:AY:416:LYS:HD3  | 24:AY:417:THR:N    | 2.15                     | 0.62              |
| 24:AY:460:GLU:O    | 24:AY:463:VAL:HB   | 2.00                     | 0.62              |
| 33:B8:14:VAL:HG21  | 33:B8:22:VAL:HG13  | 1.81                     | 0.62              |
| 35:BA:492:A:C2'    | 35:BA:493:G:H5'    | 2.30                     | 0.62              |
| 40:BF:123:LEU:HD12 | 40:BF:124:LEU:N    | 2.15                     | 0.62              |
| 40:BF:59:TYR:HE1   | 40:BF:85:GLY:O     | 1.83                     | 0.62              |
| 44:BK:17:ALA:HB3   | 44:BK:38:VAL:HG13  | 1.81                     | 0.62              |
| 35:BA:1012:U:C4    | 46:BN:28:THR:HG21  | 2.35                     | 0.62              |
| 46:BN:39:ARG:HB2   | 46:BN:41:ASP:OD1   | 1.98                     | 0.62              |
| 46:BN:48:MET:N     | 46:BN:48:MET:HE2   | 2.08                     | 0.62              |
| 52:BT:28:VAL:HG22  | 52:BT:47:GLY:N     | 2.14                     | 0.62              |
| 1:CA:999:C:H2'     | 1:CA:1000:U:C5     | 2.34                     | 0.62              |
| 3:CC:52:LEU:CD2    | 3:CC:52:LEU:H      | 2.11                     | 0.62              |
| 13:CM:63:THR:HG22  | 13:CM:64:TRP:N     | 2.14                     | 0.62              |
| 15:CO:56:LEU:O     | 15:CO:60:VAL:HG23  | 2.00                     | 0.62              |
| 24:CY:21:ILE:N     | 24:CY:21:ILE:HD13  | 2.15                     | 0.62              |
| 27:D2:39:ALA:HA    | 27:D2:45:SER:HB3   | 1.82                     | 0.62              |
| 32:D7:24:THR:HG23  | 32:D7:27:GLY:N     | 2.15                     | 0.62              |
| 35:DA:2312:U:C2'   | 35:DA:2313:C:H5''  | 2.30                     | 0.62              |
| 35:DA:271(R):G:O2' | 35:DA:271(S):G:H5' | 2.00                     | 0.62              |
| 35:DA:2876:G:H4'   | 52:DT:3:ARG:NE     | 2.12                     | 0.62              |
| 35:DA:965:C:C4'    | 35:DA:2273:A:H1'   | 2.30                     | 0.62              |
| 38:DD:24:ILE:O     | 38:DD:25:THR:O     | 2.18                     | 0.62              |
| 39:DE:78:LEU:C     | 39:DE:79:ARG:HD2   | 2.19                     | 0.62              |
| 40:DF:177:ALA:HB1  | 40:DF:178:PRO:HD2  | 1.80                     | 0.62              |
| 40:DF:123:LEU:CD1  | 40:DF:192:LEU:HD22 | 2.29                     | 0.62              |
| 42:DH:98:LEU:HD12  | 42:DH:102:ALA:O    | 2.00                     | 0.62              |
| 46:DN:23:LEU:O     | 46:DN:23:LEU:HD23  | 1.99                     | 0.62              |
| 47:DO:26:LYS:HB3   | 47:DO:30:ALA:HB2   | 1.82                     | 0.62              |
| 51:DS:89:ARG:CG    | 51:DS:92:TYR:HA    | 2.28                     | 0.62              |
| 1:AA:1275:A:O2'    | 1:AA:1276:G:H5'    | 1.99                     | 0.62              |
| 2:AB:31:TYR:CE1    | 2:AB:200:ILE:HD12  | 2.32                     | 0.62              |
| 2:AB:43:ASP:OD2    | 2:AB:46:LYS:HB2    | 2.00                     | 0.62              |
| 8:AH:120:THR:HG23  | 8:AH:123:GLU:OE1   | 1.99                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:AM:63:THR:HG22  | 13:AM:64:TRP:N     | 2.14                     | 0.62              |
| 14:AN:12:ARG:O     | 14:AN:14:PRO:HD3   | 1.98                     | 0.62              |
| 20:AT:33:ILE:HD13  | 20:AT:63:ILE:HG12  | 1.82                     | 0.62              |
| 27:B2:64:LEU:O     | 27:B2:68:ARG:HB2   | 1.99                     | 0.62              |
| 30:B5:40:LYS:HE2   | 30:B5:46:CYS:HB3   | 1.82                     | 0.62              |
| 33:B8:8:LYS:HE3    | 35:BA:245:G:O6     | 2.00                     | 0.62              |
| 35:BA:1062:G:H21   | 44:BK:133:SER:HA   | 1.63                     | 0.62              |
| 35:BA:2039:C:H2'   | 35:BA:2040:C:H6    | 1.65                     | 0.62              |
| 35:BA:2286:A:H4'   | 35:BA:2287:A:C5'   | 2.25                     | 0.62              |
| 35:BA:481:G:H2'    | 35:BA:507:A:N1     | 2.14                     | 0.62              |
| 35:BA:781:A:C8     | 38:BD:219:PRO:HG3  | 2.35                     | 0.62              |
| 38:BD:43:ARG:HD2   | 38:BD:44:ASN:OD1   | 1.99                     | 0.62              |
| 40:BF:177:ALA:HB1  | 40:BF:178:PRO:HD2  | 1.82                     | 0.62              |
| 42:BH:85:LYS:O     | 42:BH:85:LYS:HD3   | 1.99                     | 0.62              |
| 44:BK:134:MET:HG3  | 44:BK:136:VAL:HG12 | 1.82                     | 0.62              |
| 46:BN:120:LEU:HD11 | 46:BN:122:VAL:HG23 | 1.82                     | 0.62              |
| 46:BN:46:VAL:HG13  | 46:BN:47:ALA:N     | 2.08                     | 0.62              |
| 48:BP:24:GLY:CA    | 48:BP:33:ARG:NH1   | 2.63                     | 0.62              |
| 48:BP:96:THR:O     | 48:BP:99:LEU:HB3   | 1.99                     | 0.62              |
| 50:BR:18:LEU:HD23  | 50:BR:18:LEU:C     | 2.20                     | 0.62              |
| 53:BU:92:ARG:NH1   | 54:BV:11:GLN:HG3   | 2.15                     | 0.62              |
| 57:BY:23:ARG:O     | 57:BY:24:VAL:O     | 2.18                     | 0.62              |
| 1:CA:101:A:O2'     | 1:CA:102:G:H5'     | 2.00                     | 0.62              |
| 1:CA:1082:G:O2'    | 1:CA:1083:U:H5'    | 2.00                     | 0.62              |
| 1:CA:1144:G:H21    | 1:CA:1146:A:H62    | 1.48                     | 0.62              |
| 1:CA:1239:A:H62    | 1:CA:1299:A:N6     | 1.97                     | 0.62              |
| 1:CA:1279:A:H5'    | 1:CA:1280:A:OP1    | 2.00                     | 0.62              |
| 1:CA:332:G:O2'     | 1:CA:333:G:H5'     | 1.99                     | 0.62              |
| 1:CA:687:A:H62     | 1:CA:703:G:H1'     | 1.65                     | 0.62              |
| 27:D2:32:LEU:O     | 27:D2:32:LEU:HD23  | 2.00                     | 0.62              |
| 35:DA:1047:G:HO2'  | 35:DA:1110:G:H1    | 1.48                     | 0.62              |
| 35:DA:2531:A:OP1   | 42:DH:177:GLY:N    | 2.33                     | 0.62              |
| 42:DH:149:ARG:HA   | 42:DH:162:ILE:CD1  | 2.29                     | 0.62              |
| 46:DN:39:ARG:HB2   | 46:DN:41:ASP:OD1   | 2.00                     | 0.62              |
| 47:DO:18:LYS:HB2   | 47:DO:45:GLU:HG2   | 1.82                     | 0.62              |
| 53:DU:55:ARG:HA    | 53:DU:58:ARG:HG3   | 1.81                     | 0.62              |
| 1:AA:1220:G:H2'    | 1:AA:1221:G:H8     | 1.64                     | 0.61              |
| 1:AA:1294:G:O2'    | 1:AA:1295:G:H5'    | 1.99                     | 0.61              |
| 1:AA:1522:U:H2'    | 1:AA:1523:G:H8     | 1.64                     | 0.61              |
| 1:AA:539:A:H2'     | 1:AA:540:G:C8      | 2.35                     | 0.61              |
| 5:AE:36:ASP:O      | 5:AE:37:ARG:HB2    | 2.00                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1316:G:O2'    | 14:AN:18:VAL:HG11  | 2.00                     | 0.61              |
| 17:AQ:48:GLU:O     | 17:AQ:49:GLU:C     | 2.38                     | 0.61              |
| 24:AY:168:ILE:HD11 | 24:AY:178:ILE:HD11 | 1.82                     | 0.61              |
| 35:BA:139(A):G:H22 | 56:BX:44:GLU:CD    | 2.02                     | 0.61              |
| 35:BA:1887:C:H3'   | 35:BA:1888:G:H5''  | 1.80                     | 0.61              |
| 35:BA:336:C:H4'    | 57:BY:7:VAL:HG21   | 1.81                     | 0.61              |
| 35:BA:363(D):G:O2' | 35:BA:363(E):U:H5' | 2.00                     | 0.61              |
| 35:BA:742:G:O2'    | 35:BA:743:G:H5'    | 1.99                     | 0.61              |
| 35:BA:322:A:H3'    | 40:BF:169:ASN:HD21 | 1.64                     | 0.61              |
| 46:BN:14:VAL:HG11  | 46:BN:137:LYS:HD2  | 1.80                     | 0.61              |
| 48:BP:102:ARG:HB3  | 48:BP:102:ARG:CZ   | 2.30                     | 0.61              |
| 50:BR:99:LYS:CD    | 50:BR:99:LYS:H     | 1.89                     | 0.61              |
| 36:BB:7:G:H5'      | 51:BS:29:PHE:CE1   | 2.34                     | 0.61              |
| 51:BS:89:ARG:CG    | 51:BS:92:TYR:HA    | 2.30                     | 0.61              |
| 52:BT:91:ARG:O     | 52:BT:117:ASP:HB2  | 2.00                     | 0.61              |
| 52:BT:38:ASN:ND2   | 52:BT:40:THR:H     | 1.97                     | 0.61              |
| 56:BX:36:LYS:HB3   | 56:BX:56:THR:HG21  | 1.82                     | 0.61              |
| 57:BY:27:VAL:HG12  | 57:BY:29:GLU:OE1   | 1.99                     | 0.61              |
| 1:CA:1160:G:O6     | 1:CA:1181:G:O6     | 2.18                     | 0.61              |
| 1:CA:820:U:H4'     | 1:CA:821:G:OP2     | 1.99                     | 0.61              |
| 1:CA:943:U:C2'     | 1:CA:944:G:H5'     | 2.30                     | 0.61              |
| 2:CB:194:PRO:O     | 2:CB:197:VAL:HG23  | 2.00                     | 0.61              |
| 11:CK:59:TYR:O     | 11:CK:62:GLN:HB3   | 2.00                     | 0.61              |
| 15:CO:83:GLU:C     | 15:CO:85:LEU:H     | 2.03                     | 0.61              |
| 24:CY:84:THR:N     | 24:CY:85:PRO:CD    | 2.62                     | 0.61              |
| 33:D8:61:LEU:CD1   | 33:D8:62:LEU:H     | 2.09                     | 0.61              |
| 35:DA:1775:U:C2'   | 35:DA:1776:G:H5'   | 2.30                     | 0.61              |
| 35:DA:1942:C:H3'   | 35:DA:1943:U:H5''  | 1.81                     | 0.61              |
| 35:DA:608:A:H2'    | 35:DA:609:A:C8     | 2.35                     | 0.61              |
| 36:DB:68:C:H2'     | 36:DB:69:G:H8      | 1.65                     | 0.61              |
| 37:DC:132:LEU:HB3  | 37:DC:138:LEU:N    | 2.15                     | 0.61              |
| 39:DE:77:ILE:HG22  | 39:DE:78:LEU:CD1   | 2.29                     | 0.61              |
| 46:DN:46:VAL:HG13  | 46:DN:47:ALA:N     | 2.08                     | 0.61              |
| 52:DT:65:LYS:CE    | 52:DT:66:VAL:H     | 2.07                     | 0.61              |
| 1:AA:1002:G:H22    | 1:AA:1039:C:H2'    | 1.64                     | 0.61              |
| 1:AA:773:G:O2'     | 1:AA:774:G:H5'     | 1.99                     | 0.61              |
| 1:AA:943:U:H2'     | 1:AA:944:G:H5'     | 1.81                     | 0.61              |
| 9:AI:104:ARG:C     | 9:AI:105:ASP:N     | 2.54                     | 0.61              |
| 10:AJ:30:SER:OG    | 10:AJ:81:THR:HG22  | 2.00                     | 0.61              |
| 11:AK:34:ASP:HB2   | 11:AK:35:PRO:CD    | 2.29                     | 0.61              |
| 15:AO:17:ARG:HD3   | 15:AO:26:GLU:HG3   | 1.82                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:AT:42:GLN:HE21  | 20:AT:42:GLN:HA    | 1.65                     | 0.61              |
| 24:AY:117:GLN:HE22 | 24:AY:120:THR:HG23 | 1.65                     | 0.61              |
| 24:AY:491:VAL:HG12 | 24:AY:492:ASP:N    | 2.15                     | 0.61              |
| 24:AY:647:VAL:HG21 | 24:AY:652:MET:SD   | 2.40                     | 0.61              |
| 24:AY:655:TYR:OH   | 24:AY:659:LEU:HD23 | 1.99                     | 0.61              |
| 35:BA:1075:C:H5'   | 35:BA:1076:C:OP2   | 2.00                     | 0.61              |
| 35:BA:1885:A:H8    | 35:BA:1885:A:H5'   | 1.65                     | 0.61              |
| 35:BA:2712:U:HO2'  | 35:BA:2712(A):A:H8 | 0.72                     | 0.61              |
| 35:BA:2774:C:H2'   | 35:BA:2775:A:O4'   | 2.00                     | 0.61              |
| 35:BA:52:A:O2'     | 35:BA:53:A:H5'     | 2.01                     | 0.61              |
| 35:BA:650:C:H2'    | 35:BA:651:G:H5''   | 1.82                     | 0.61              |
| 39:BE:4:ILE:HG13   | 39:BE:5:LEU:N      | 2.15                     | 0.61              |
| 48:BP:83:VAL:H     | 48:BP:115:LEU:CD2  | 2.12                     | 0.61              |
| 51:BS:98:VAL:HG12  | 51:BS:100:ALA:HB2  | 1.82                     | 0.61              |
| 51:BS:15:ARG:HB3   | 51:BS:18:ILE:CD1   | 2.28                     | 0.61              |
| 1:CA:1119:C:O2'    | 1:CA:1120:G:H5'    | 2.00                     | 0.61              |
| 1:CA:161:A:H2'     | 1:CA:162:A:H8      | 1.65                     | 0.61              |
| 24:CY:14:ASN:HB2   | 24:CY:102:ASP:OD1  | 2.00                     | 0.61              |
| 24:CY:580:MET:O    | 24:CY:584:ILE:HG12 | 2.00                     | 0.61              |
| 24:CY:605:ILE:CD1  | 24:CY:677:GLN:HG2  | 2.29                     | 0.61              |
| 35:DA:1068:G:H21   | 35:DA:1096:A:H5'   | 1.64                     | 0.61              |
| 35:DA:1541:G:O2'   | 35:DA:1542:A:H5''  | 2.00                     | 0.61              |
| 35:DA:1815:A:OP2   | 35:DA:1822:G:H5''  | 2.00                     | 0.61              |
| 35:DA:1887:C:H3'   | 35:DA:1888:G:H5''  | 1.80                     | 0.61              |
| 35:DA:1921:G:O2'   | 35:DA:1922:G:H5'   | 2.00                     | 0.61              |
| 35:DA:406:G:HO2'   | 35:DA:407:G:H8     | 1.48                     | 0.61              |
| 38:DD:153:ALA:O    | 38:DD:154:LYS:HG3  | 1.99                     | 0.61              |
| 39:DE:9:VAL:CG2    | 39:DE:10:GLY:N     | 2.63                     | 0.61              |
| 39:DE:101:ARG:HH11 | 39:DE:169:ASN:HD22 | 1.47                     | 0.61              |
| 39:DE:101:ARG:NH1  | 39:DE:169:ASN:HD22 | 1.97                     | 0.61              |
| 40:DF:133:ASN:H    | 40:DF:162:LEU:HD23 | 1.65                     | 0.61              |
| 51:DS:97:ARG:C     | 51:DS:97:ARG:NE    | 2.53                     | 0.61              |
| 35:DA:583:G:OP2    | 53:DU:10:ARG:HD2   | 2.00                     | 0.61              |
| 57:DY:8:LYS:HE2    | 57:DY:72:VAL:HG23  | 1.82                     | 0.61              |
| 1:AA:723:U:H5'     | 1:AA:724:G:OP2     | 2.00                     | 0.61              |
| 1:AA:740:U:O2'     | 1:AA:741:G:H5'     | 2.00                     | 0.61              |
| 2:AB:32:ILE:HD11   | 2:AB:40:HIS:HB3    | 1.82                     | 0.61              |
| 9:AI:47:LEU:N      | 9:AI:47:LEU:CD1    | 2.63                     | 0.61              |
| 12:AL:126:LYS:HG3  | 12:AL:128:ALA:H    | 1.64                     | 0.61              |
| 22:AW:18:U:H2'     | 22:AW:19:G:H5''    | 1.80                     | 0.61              |
| 24:AY:630:GLN:HE22 | 24:AY:646:PHE:HD2  | 1.48                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:1163:G:O2'   | 35:BA:1164:G:H5'   | 2.00                     | 0.61              |
| 35:BA:1504:C:C2'   | 35:BA:1505:C:H5''  | 2.30                     | 0.61              |
| 35:BA:1943:U:H2'   | 35:BA:1943:U:O2    | 2.00                     | 0.61              |
| 35:BA:2200:C:H42   | 35:BA:2223:G:H1    | 1.48                     | 0.61              |
| 35:BA:2312:U:C2'   | 35:BA:2313:C:H5''  | 2.30                     | 0.61              |
| 35:BA:271(R):G:O2' | 35:BA:271(S):G:H5' | 2.00                     | 0.61              |
| 35:BA:311:A:H5'    | 35:BA:332:A:C2     | 2.36                     | 0.61              |
| 39:BE:7:VAL:HG12   | 39:BE:27:LEU:HB3   | 1.80                     | 0.61              |
| 41:BG:111:LEU:HA   | 41:BG:114:ILE:HD11 | 1.82                     | 0.61              |
| 42:BH:19:VAL:HG12  | 42:BH:20:ALA:N     | 2.14                     | 0.61              |
| 42:BH:44:VAL:O     | 42:BH:46:GLU:HG2   | 2.00                     | 0.61              |
| 47:BO:91:LEU:N     | 47:BO:91:LEU:HD22  | 2.15                     | 0.61              |
| 50:BR:117:VAL:CG1  | 50:BR:118:GLU:N    | 2.64                     | 0.61              |
| 54:BV:18:LEU:HD13  | 54:BV:19:LYS:N     | 2.15                     | 0.61              |
| 57:BY:55:TYR:CD2   | 57:BY:55:TYR:N     | 2.68                     | 0.61              |
| 57:BY:55:TYR:HD2   | 57:BY:55:TYR:N     | 1.98                     | 0.61              |
| 58:BZ:167:PRO:O    | 58:BZ:168:GLU:HB2  | 2.00                     | 0.61              |
| 1:CA:1319:A:OP1    | 19:CS:10:PHE:CE1   | 2.53                     | 0.61              |
| 1:CA:189:G:H2'     | 1:CA:189(A):C:C6   | 2.35                     | 0.61              |
| 1:CA:192:U:H2'     | 1:CA:193:C:C6      | 2.35                     | 0.61              |
| 1:CA:812:C:HO2'    | 1:CA:813:U:P       | 2.23                     | 0.61              |
| 3:CC:70:VAL:CG1    | 3:CC:71:ALA:N      | 2.62                     | 0.61              |
| 4:CD:126:ILE:HD12  | 4:CD:126:ILE:N     | 2.15                     | 0.61              |
| 4:CD:92:VAL:O      | 4:CD:96:LEU:HD22   | 2.00                     | 0.61              |
| 9:CI:5:TYR:CD2     | 9:CI:6:GLY:N       | 2.65                     | 0.61              |
| 12:CL:28:LYS:O     | 12:CL:29:GLY:C     | 2.38                     | 0.61              |
| 19:CS:6:LYS:HG2    | 19:CS:7:LYS:CE     | 2.29                     | 0.61              |
| 24:CY:181:LEU:HD11 | 24:CY:242:LEU:HB3  | 1.81                     | 0.61              |
| 24:CY:546:ILE:CG2  | 24:CY:590:ILE:HG13 | 2.21                     | 0.61              |
| 24:CY:71:THR:HB    | 24:CY:78:ARG:NH1   | 2.15                     | 0.61              |
| 33:D8:61:LEU:C     | 33:D8:63:PRO:HD2   | 2.20                     | 0.61              |
| 35:DA:1649:G:O2'   | 35:DA:1650:G:H5'   | 2.00                     | 0.61              |
| 35:DA:2523:G:H2'   | 35:DA:2524:G:C5'   | 2.26                     | 0.61              |
| 35:DA:2672:G:C3'   | 35:DA:2673:G:H5''  | 2.30                     | 0.61              |
| 35:DA:55:G:H2'     | 35:DA:56:A:H8      | 1.64                     | 0.61              |
| 37:DC:191:ARG:HH11 | 37:DC:191:ARG:HG3  | 1.64                     | 0.61              |
| 41:DG:68:PRO:HA    | 41:DG:92:VAL:HG11  | 1.82                     | 0.61              |
| 41:DG:9:ARG:HG2    | 41:DG:13:GLU:OE1   | 2.00                     | 0.61              |
| 35:DA:2531:A:OP1   | 42:DH:177:GLY:C    | 2.39                     | 0.61              |
| 42:DH:65:HIS:HE1   | 42:DH:69:ARG:HH11  | 1.46                     | 0.61              |
| 48:DP:83:VAL:H     | 48:DP:115:LEU:CD2  | 2.13                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 52:DT:50:ILE:N      | 52:DT:50:ILE:HD12  | 2.15                     | 0.61              |
| 57:DY:55:TYR:HD2    | 57:DY:55:TYR:N     | 1.98                     | 0.61              |
| 49:DQ:63:LYS:HA     | 58:DZ:178:GLU:OE1  | 1.99                     | 0.61              |
| 58:DZ:9:TYR:CE2     | 58:DZ:61:LEU:HD22  | 2.33                     | 0.61              |
| 1:AA:59:A:N3        | 1:AA:59:A:H2'      | 2.14                     | 0.61              |
| 9:AI:4:TYR:CE2      | 9:AI:88:TYR:HB2    | 2.35                     | 0.61              |
| 10:AJ:61:GLU:OE2    | 14:AN:45:ARG:HD2   | 2.00                     | 0.61              |
| 11:AK:18:ARG:HH21   | 11:AK:37:GLY:N     | 1.98                     | 0.61              |
| 22:AW:17:C:H5'      | 22:AW:62:C:OP1     | 2.01                     | 0.61              |
| 22:AW:37:U:H3       | 23:AX:13:A:N6      | 1.98                     | 0.61              |
| 24:AY:337:SER:HA    | 24:AY:355:LEU:HD23 | 1.80                     | 0.61              |
| 24:AY:603:GLU:O     | 24:AY:676:TYR:HA   | 2.00                     | 0.61              |
| 30:B5:19:ARG:HA     | 35:BA:2046:G:C5'   | 2.29                     | 0.61              |
| 30:B5:36:CYS:SG     | 30:B5:38:ALA:HB3   | 2.40                     | 0.61              |
| 35:BA:1068:G:H21    | 35:BA:1096:A:H5'   | 1.65                     | 0.61              |
| 35:BA:1142(A):A:O2' | 35:BA:1143:A:H5''  | 2.00                     | 0.61              |
| 35:BA:1510:G:O2'    | 35:BA:1511:C:H5'   | 2.00                     | 0.61              |
| 35:BA:1775:U:H2'    | 35:BA:1776:G:C5'   | 2.30                     | 0.61              |
| 25:B0:16:SER:HB2    | 35:BA:2262:U:C5    | 2.34                     | 0.61              |
| 48:BP:124:LYS:HD3   | 48:BP:143:GLY:HA3  | 1.81                     | 0.61              |
| 52:BT:35:LYS:NZ     | 52:BT:41:ARG:HH11  | 1.98                     | 0.61              |
| 55:BW:9:TYR:H       | 55:BW:102:HIS:HD2  | 1.48                     | 0.61              |
| 35:BA:480:A:OP2     | 57:BY:46:LYS:HE2   | 2.00                     | 0.61              |
| 5:CE:36:ASP:OD1     | 5:CE:38:GLN:N      | 2.26                     | 0.61              |
| 9:CI:4:TYR:CE2      | 9:CI:88:TYR:HB2    | 2.36                     | 0.61              |
| 12:CL:126:LYS:HG3   | 12:CL:128:ALA:H    | 1.64                     | 0.61              |
| 1:CA:254:G:OP1      | 17:CQ:67:LYS:O     | 2.18                     | 0.61              |
| 22:CV:21:A:N6       | 22:CV:46:G:H2'     | 2.14                     | 0.61              |
| 24:CY:416:LYS:HG2   | 24:CY:417:THR:H    | 1.64                     | 0.61              |
| 35:DA:1516:C:H2'    | 35:DA:1517:G:C5'   | 2.30                     | 0.61              |
| 35:DA:1827:C:O2'    | 35:DA:1828:G:H5'   | 1.99                     | 0.61              |
| 35:DA:286:C:H2'     | 35:DA:287:C:C6     | 2.35                     | 0.61              |
| 35:DA:364:C:H2'     | 35:DA:365:C:C5'    | 2.30                     | 0.61              |
| 35:DA:603:A:H4'     | 35:DA:604:G:O5'    | 1.99                     | 0.61              |
| 37:DC:115:VAL:HA    | 37:DC:145:THR:HG22 | 1.82                     | 0.61              |
| 39:DE:4:ILE:HG13    | 39:DE:5:LEU:N      | 2.16                     | 0.61              |
| 35:DA:1062:G:H21    | 44:DK:133:SER:HA   | 1.65                     | 0.61              |
| 44:DK:134:MET:HG3   | 44:DK:136:VAL:HG12 | 1.81                     | 0.61              |
| 48:DP:91:PHE:N      | 48:DP:91:PHE:CD1   | 2.69                     | 0.61              |
| 52:DT:42:ILE:HG13   | 52:DT:42:ILE:O     | 2.00                     | 0.61              |
| 52:DT:91:ARG:O      | 52:DT:117:ASP:HB2  | 2.00                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:DY:55:TYR:CD2   | 57:DY:55:TYR:N     | 2.69                     | 0.61              |
| 2:AB:61:LEU:HD23   | 2:AB:68:ILE:HD11   | 1.83                     | 0.61              |
| 4:AD:10:ARG:O      | 4:AD:13:ARG:HB2    | 1.99                     | 0.61              |
| 4:AD:26:CYS:HA     | 4:AD:31:CYS:HA     | 1.83                     | 0.61              |
| 6:AF:36:ARG:CZ     | 6:AF:36:ARG:HB3    | 2.30                     | 0.61              |
| 20:AT:29:LYS:O     | 20:AT:33:ILE:HG13  | 2.00                     | 0.61              |
| 24:AY:443:HIS:CE1  | 24:AY:445:GLU:HB2  | 2.36                     | 0.61              |
| 61:AY:702:FUA:O2   | 61:AY:702:FUA:H211 | 2.00                     | 0.61              |
| 25:B0:24:LYS:O     | 25:B0:25:ARG:HD3   | 2.01                     | 0.61              |
| 35:BA:1516:C:C2'   | 35:BA:1517:G:H5''  | 2.30                     | 0.61              |
| 35:BA:1523:U:H2'   | 35:BA:1524:G:C8    | 2.35                     | 0.61              |
| 35:BA:1578:U:C2'   | 35:BA:1579:A:H5''  | 2.31                     | 0.61              |
| 35:BA:1748:G:H2'   | 35:BA:1749:A:O4'   | 2.00                     | 0.61              |
| 35:BA:570:G:H2'    | 35:BA:2030:A:N7    | 2.16                     | 0.61              |
| 35:BA:528:A:H2     | 35:BA:2043:C:C4'   | 2.13                     | 0.61              |
| 35:BA:2345:G:O2'   | 35:BA:2381:C:H2'   | 2.00                     | 0.61              |
| 35:BA:2443:C:H2'   | 35:BA:2443:C:O2    | 2.00                     | 0.61              |
| 35:BA:2672:G:C3'   | 35:BA:2673:G:H5''  | 2.30                     | 0.61              |
| 35:BA:272(B):G:H2' | 35:BA:272(C):G:C8  | 2.34                     | 0.61              |
| 35:BA:422:A:H2'    | 35:BA:423:A:C8     | 2.35                     | 0.61              |
| 36:BB:54:G:O2'     | 36:BB:55:U:H5'     | 2.00                     | 0.61              |
| 38:BD:11:PRO:C     | 38:BD:13:ARG:H     | 2.04                     | 0.61              |
| 39:BE:184:VAL:O    | 39:BE:186:GLY:N    | 2.29                     | 0.61              |
| 39:BE:78:LEU:C     | 39:BE:79:ARG:HD2   | 2.20                     | 0.61              |
| 40:BF:16:GLY:O     | 40:BF:17:ARG:HG3   | 2.00                     | 0.61              |
| 45:BL:100:UNK:O    | 45:BL:101:UNK:CB   | 2.49                     | 0.61              |
| 47:BO:64:ARG:O     | 47:BO:82:ASN:HA    | 2.00                     | 0.61              |
| 47:BO:87:ILE:HD13  | 47:BO:87:ILE:N     | 2.15                     | 0.61              |
| 50:BR:45:ARG:HG3   | 50:BR:46:GLY:N     | 2.12                     | 0.61              |
| 1:CA:1423:G:C5'    | 47:DO:49:ARG:HH22  | 2.14                     | 0.61              |
| 1:CA:22:G:O2'      | 1:CA:23:C:H5'      | 2.01                     | 0.61              |
| 1:CA:954:G:H2'     | 1:CA:955:U:C6      | 2.35                     | 0.61              |
| 13:CM:4:ILE:HG22   | 13:CM:5:ALA:N      | 2.14                     | 0.61              |
| 19:CS:31:ILE:HG23  | 19:CS:49:ILE:HG23  | 1.83                     | 0.61              |
| 24:CY:355:LEU:HD12 | 24:CY:369:LEU:HD13 | 1.81                     | 0.61              |
| 24:CY:510:VAL:CG1  | 24:CY:567:LEU:HD13 | 2.30                     | 0.61              |
| 35:DA:11:G:H2'     | 35:DA:12:U:C6      | 2.35                     | 0.61              |
| 35:DA:2040:C:H2'   | 35:DA:2041:U:C6    | 2.36                     | 0.61              |
| 35:DA:2286:A:H4'   | 35:DA:2287:A:C5'   | 2.26                     | 0.61              |
| 35:DA:764:A:N3     | 38:DD:213:ARG:NH1  | 2.49                     | 0.61              |
| 38:DD:241:PRO:C    | 38:DD:242:ARG:HG3  | 2.20                     | 0.61              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:DF:89:VAL:HG12  | 40:DF:90:PHE:H    | 1.65                     | 0.61              |
| 47:DO:97:ARG:HG3   | 47:DO:97:ARG:HH11 | 1.64                     | 0.61              |
| 48:DP:80:TYR:CD1   | 48:DP:111:ARG:HB3 | 2.35                     | 0.61              |
| 49:DQ:56:ARG:HA    | 49:DQ:56:ARG:HE   | 1.65                     | 0.61              |
| 51:DS:98:VAL:HG12  | 51:DS:100:ALA:N   | 2.16                     | 0.61              |
| 51:DS:19:LYS:O     | 51:DS:20:ARG:NH2  | 2.33                     | 0.61              |
| 52:DT:35:LYS:NZ    | 52:DT:41:ARG:NH1  | 2.47                     | 0.61              |
| 56:DX:36:LYS:HB3   | 56:DX:56:THR:HG21 | 1.83                     | 0.61              |
| 1:AA:1269:A:C2     | 1:AA:1313:U:O4'   | 2.53                     | 0.61              |
| 1:AA:1348:U:H4'    | 9:AI:120:ARG:HG3  | 1.82                     | 0.61              |
| 1:AA:160:A:H1'     | 1:AA:344:A:C8     | 2.35                     | 0.61              |
| 3:AC:150:LYS:HB2   | 3:AC:169:ALA:HB2  | 1.83                     | 0.61              |
| 3:AC:142:MET:CE    | 3:AC:171:GLY:HA3  | 2.30                     | 0.61              |
| 19:AS:14:HIS:CD2   | 19:AS:15:LEU:HD23 | 2.36                     | 0.61              |
| 24:AY:67:ALA:HB1   | 24:AY:327:PHE:HZ  | 1.66                     | 0.61              |
| 24:AY:491:VAL:HG12 | 24:AY:492:ASP:H   | 1.65                     | 0.61              |
| 33:B8:47:LYS:NZ    | 33:B8:49:VAL:HG13 | 2.15                     | 0.61              |
| 33:B8:6:THR:HG22   | 33:B8:63:PRO:HD3  | 1.81                     | 0.61              |
| 35:BA:2037:G:H2'   | 35:BA:2038:G:C8   | 2.36                     | 0.61              |
| 35:BA:30:G:O2'     | 35:BA:31:C:H5'    | 2.00                     | 0.61              |
| 38:BD:146:GLU:HG2  | 38:BD:152:GLY:C   | 2.20                     | 0.61              |
| 39:BE:8:LYS:O      | 39:BE:193:GLY:N   | 2.31                     | 0.61              |
| 41:BG:98:ARG:CG    | 41:BG:98:ARG:HH11 | 2.13                     | 0.61              |
| 44:BK:37:PHE:O     | 44:BK:41:PHE:HB3  | 2.01                     | 0.61              |
| 46:BN:133:GLN:HG2  | 46:BN:134:ARG:N   | 2.16                     | 0.61              |
| 47:BO:47:ILE:HG22  | 47:BO:48:PRO:HD2  | 1.82                     | 0.61              |
| 50:BR:78:LYS:O     | 50:BR:83:ILE:HG12 | 2.01                     | 0.61              |
| 51:BS:19:LYS:O     | 51:BS:20:ARG:NH2  | 2.33                     | 0.61              |
| 58:BZ:3:TYR:CE2    | 58:BZ:51:ALA:HB2  | 2.36                     | 0.61              |
| 1:CA:1128:C:H2'    | 1:CA:1129:C:C5'   | 2.25                     | 0.61              |
| 1:CA:301:G:O2'     | 1:CA:302:G:H5'    | 2.00                     | 0.61              |
| 4:CD:61:LYS:HD3    | 4:CD:206:PHE:CE2  | 2.35                     | 0.61              |
| 9:CI:104:ARG:C     | 9:CI:105:ASP:N    | 2.54                     | 0.61              |
| 13:CM:10:PRO:HG2   | 13:CM:11:ARG:H    | 1.65                     | 0.61              |
| 13:CM:74:VAL:HA    | 13:CM:77:ASN:HD22 | 1.64                     | 0.61              |
| 24:CY:553:GLY:N    | 24:CY:557:GLY:HA2 | 2.15                     | 0.61              |
| 31:D6:15:GLU:CG    | 31:D6:47:THR:HG21 | 2.31                     | 0.61              |
| 35:DA:1114:G:H2'   | 35:DA:1115:G:H5'  | 1.82                     | 0.61              |
| 35:DA:1389:G:H2'   | 35:DA:1390:U:C6   | 2.36                     | 0.61              |
| 35:DA:2603:G:O2'   | 35:DA:2604:U:H5'  | 2.01                     | 0.61              |
| 35:DA:759:G:H2'    | 35:DA:760:G:H8    | 1.64                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:DC:101:ILE:HD12 | 37:DC:101:ILE:H    | 1.65                     | 0.61              |
| 37:DC:73:VAL:HG11  | 37:DC:158:LYS:HA   | 1.83                     | 0.61              |
| 35:DA:2175:C:H1'   | 37:DC:218:THR:O    | 1.99                     | 0.61              |
| 38:DD:10:THR:HG23  | 38:DD:13:ARG:HB3   | 1.81                     | 0.61              |
| 38:DD:166:GLN:HE21 | 38:DD:166:GLN:HA   | 1.66                     | 0.61              |
| 42:DH:44:VAL:O     | 42:DH:46:GLU:HG2   | 2.01                     | 0.61              |
| 48:DP:102:ARG:HB3  | 48:DP:102:ARG:CZ   | 2.30                     | 0.61              |
| 49:DQ:43:THR:O     | 49:DQ:47:ILE:HG13  | 2.00                     | 0.61              |
| 52:DT:65:LYS:HZ1   | 52:DT:65:LYS:HA    | 1.65                     | 0.61              |
| 1:AA:1160:G:O6     | 1:AA:1181:G:O6     | 2.18                     | 0.61              |
| 1:AA:1347:G:H3'    | 9:AI:108:VAL:O     | 2.00                     | 0.61              |
| 1:AA:673:G:H2'     | 1:AA:674:G:C8      | 2.35                     | 0.61              |
| 4:AD:126:ILE:HD12  | 4:AD:126:ILE:N     | 2.16                     | 0.61              |
| 4:AD:58:LEU:HD23   | 4:AD:58:LEU:C      | 2.21                     | 0.61              |
| 5:AE:64:ARG:HH11   | 5:AE:64:ARG:CG     | 2.11                     | 0.61              |
| 12:AL:69:TYR:O     | 12:AL:71:PRO:HD3   | 2.00                     | 0.61              |
| 13:AM:83:ASP:CG    | 13:AM:84:ILE:H     | 2.03                     | 0.61              |
| 16:AP:14:ASN:N     | 16:AP:15:PRO:HD3   | 2.15                     | 0.61              |
| 17:AQ:57:VAL:HG23  | 17:AQ:58:GLU:N     | 2.16                     | 0.61              |
| 24:AY:402:ILE:HD12 | 24:AY:402:ILE:H    | 1.65                     | 0.61              |
| 24:AY:457:LEU:O    | 24:AY:461:ILE:HG13 | 2.01                     | 0.61              |
| 24:AY:84:THR:O     | 24:AY:85:PRO:C     | 2.39                     | 0.61              |
| 26:B1:56:GLN:OE1   | 26:B1:85:LEU:HD23  | 2.01                     | 0.61              |
| 31:B6:28:ARG:CB    | 31:B6:28:ARG:HH11  | 2.13                     | 0.61              |
| 35:BA:1326:U:O2'   | 35:BA:1327:C:H5'   | 2.01                     | 0.61              |
| 35:BA:1389:G:H2'   | 35:BA:1390:U:C6    | 2.35                     | 0.61              |
| 35:BA:1504:C:C3'   | 35:BA:1505:C:H5''  | 2.31                     | 0.61              |
| 35:BA:2454:G:O2'   | 35:BA:2455:G:H5'   | 2.01                     | 0.61              |
| 35:BA:272(J):C:C3' | 35:BA:274:G:H5''   | 2.26                     | 0.61              |
| 35:BA:2839:G:H1    | 35:BA:2878:U:H3    | 1.49                     | 0.61              |
| 36:BB:68:C:H2'     | 36:BB:69:G:H8      | 1.65                     | 0.61              |
| 37:BC:101:ILE:H    | 37:BC:101:ILE:HD12 | 1.66                     | 0.61              |
| 38:BD:267:SER:HA   | 38:BD:270:ILE:HD11 | 1.83                     | 0.61              |
| 40:BF:7:TYR:HD2    | 40:BF:16:GLY:CA    | 2.13                     | 0.61              |
| 41:BG:157:ILE:HG22 | 41:BG:158:ALA:N    | 2.14                     | 0.61              |
| 41:BG:56:ALA:HA    | 41:BG:59:GLU:OE1   | 1.99                     | 0.61              |
| 49:BQ:27:VAL:HG12  | 49:BQ:28:ALA:N     | 2.16                     | 0.61              |
| 52:BT:29:ARG:HD3   | 52:BT:86:ILE:HG22  | 1.82                     | 0.61              |
| 1:CA:1208:C:H2'    | 1:CA:1209:C:C6     | 2.36                     | 0.61              |
| 1:CA:513:C:O2'     | 1:CA:514:C:H5'     | 2.01                     | 0.61              |
| 6:CF:68:PRO:HG2    | 6:CF:71:ARG:HB2    | 1.82                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1124:G:H5'    | 10:CJ:35:SER:HB2   | 1.82                     | 0.61              |
| 12:CL:34:ARG:HG3   | 12:CL:105:TYR:CE1  | 2.36                     | 0.61              |
| 22:CW:14:A:H3'     | 22:CW:15:G:H5''    | 1.83                     | 0.61              |
| 24:CY:117:GLN:NE2  | 24:CY:120:THR:HG23 | 2.15                     | 0.61              |
| 28:D3:4:LEU:HD11   | 28:D3:39:ASP:OD1   | 2.00                     | 0.61              |
| 30:D5:40:LYS:HZ3   | 30:D5:46:CYS:H     | 1.47                     | 0.61              |
| 31:D6:28:ARG:CB    | 31:D6:28:ARG:HH11  | 2.13                     | 0.61              |
| 35:DA:1416:G:HO2'  | 35:DA:1417:C:H5    | 1.48                     | 0.61              |
| 35:DA:184:C:H2'    | 35:DA:185:U:H6     | 1.63                     | 0.61              |
| 38:DD:11:PRO:O     | 38:DD:13:ARG:N     | 2.33                     | 0.61              |
| 46:DN:41:ASP:C     | 53:DU:64:ARG:HH22  | 2.03                     | 0.61              |
| 51:DS:88:ASP:CG    | 51:DS:89:ARG:N     | 2.54                     | 0.61              |
| 35:DA:1322:A:OP1   | 55:DW:11:ARG:HG3   | 2.01                     | 0.61              |
| 57:DY:23:ARG:O     | 57:DY:24:VAL:O     | 2.18                     | 0.61              |
| 1:AA:1524:C:H2'    | 1:AA:1525:G:C8     | 2.36                     | 0.61              |
| 1:AA:943:U:C2'     | 1:AA:944:G:H5'     | 2.30                     | 0.61              |
| 1:AA:974:A:H8      | 1:AA:974:A:OP1     | 1.82                     | 0.61              |
| 2:AB:194:PRO:O     | 2:AB:197:VAL:HG23  | 2.00                     | 0.61              |
| 22:AW:37:U:H3      | 23:AX:13:A:H62     | 1.49                     | 0.61              |
| 24:AY:530:VAL:HG13 | 24:AY:531:GLY:N    | 2.16                     | 0.61              |
| 30:B5:48:GLU:O     | 30:B5:49:CYS:CB    | 2.49                     | 0.61              |
| 25:B0:43:THR:HG22  | 35:BA:2331:G:O3'   | 1.99                     | 0.61              |
| 35:BA:240:G:C3'    | 35:BA:241:A:H5''   | 2.29                     | 0.61              |
| 35:BA:2832:U:H1'   | 35:BA:2834:G:C2    | 2.36                     | 0.61              |
| 37:BC:138:LEU:HD22 | 37:BC:139:PRO:HD2  | 1.83                     | 0.61              |
| 37:BC:211:ARG:HG3  | 37:BC:211:ARG:HH11 | 1.66                     | 0.61              |
| 40:BF:28:ILE:O     | 40:BF:30:PRO:HD3   | 2.00                     | 0.61              |
| 49:BQ:59:ARG:HB3   | 58:BZ:180:VAL:CG2  | 2.31                     | 0.61              |
| 1:CA:487:A:H2'     | 1:CA:488:C:O4'     | 2.01                     | 0.61              |
| 2:CB:31:TYR:CE1    | 2:CB:200:ILE:HD12  | 2.34                     | 0.61              |
| 12:CL:47:LYS:HB3   | 12:CL:48:PRO:HD3   | 1.83                     | 0.61              |
| 24:CY:491:VAL:CG1  | 24:CY:492:ASP:H    | 2.12                     | 0.61              |
| 24:CY:66:THR:O     | 24:CY:67:ALA:HB2   | 2.00                     | 0.61              |
| 29:D4:2:LYS:HG2    | 36:DB:44:G:OP2     | 2.01                     | 0.61              |
| 29:D4:56:VAL:O     | 29:D4:57:GLU:HB2   | 1.99                     | 0.61              |
| 30:D5:40:LYS:HD3   | 30:D5:44:THR:HB    | 1.83                     | 0.61              |
| 31:D6:35:GLU:HB3   | 31:D6:51:GLU:HB2   | 1.83                     | 0.61              |
| 31:D6:54:ILE:HD13  | 35:DA:2420:C:H4'   | 1.82                     | 0.61              |
| 35:DA:1064:C:H4'   | 44:DK:89:HIS:HD2   | 1.64                     | 0.61              |
| 35:DA:1094:U:H2'   | 35:DA:1096:A:OP2   | 2.01                     | 0.61              |
| 35:DA:1441:G:H2'   | 35:DA:1442:G:H8    | 1.64                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:DA:1638:C:H2'   | 35:DA:1639:U:O4'  | 2.01                     | 0.61              |
| 35:DA:1930:G:O2'   | 35:DA:1931:U:P    | 2.57                     | 0.61              |
| 35:DA:693:C:O2'    | 35:DA:694:U:H5'   | 2.01                     | 0.61              |
| 27:D2:58:ALA:CB    | 35:DA:76:C:H4'    | 2.31                     | 0.61              |
| 42:DH:86:GLU:HA    | 42:DH:132:ARG:HA  | 1.82                     | 0.61              |
| 42:DH:169:VAL:HG22 | 42:DH:170:ARG:N   | 2.12                     | 0.61              |
| 42:DH:30:LYS:CD    | 42:DH:81:GLU:HG2  | 2.30                     | 0.61              |
| 48:DP:9:ASN:H      | 48:DP:10:PRO:HD2  | 1.65                     | 0.61              |
| 35:DA:252:G:OP2    | 48:DP:50:ARG:NH1  | 2.34                     | 0.61              |
| 51:DS:89:ARG:HH11  | 51:DS:89:ARG:HG2  | 1.66                     | 0.61              |
| 53:DU:19:LYS:HB3   | 53:DU:20:LEU:HD22 | 1.82                     | 0.61              |
| 55:DW:109:GLU:CD   | 55:DW:109:GLU:H   | 2.04                     | 0.61              |
| 57:DY:31:LEU:HB2   | 57:DY:32:PRO:CA   | 2.31                     | 0.61              |
| 1:AA:100:C:H2'     | 1:AA:101:A:C8     | 2.36                     | 0.61              |
| 1:AA:101:A:O2'     | 1:AA:102:G:H5'    | 2.00                     | 0.61              |
| 4:AD:107:ARG:HH21  | 4:AD:194:LEU:CD1  | 2.14                     | 0.61              |
| 4:AD:176:LEU:HD12  | 4:AD:177:ASP:H    | 1.66                     | 0.61              |
| 5:AE:43:LEU:HD21   | 5:AE:132:ALA:HB1  | 1.82                     | 0.61              |
| 5:AE:60:TYR:CE1    | 5:AE:64:ARG:NH2   | 2.68                     | 0.61              |
| 12:AL:119:LYS:O    | 12:AL:120:TYR:HB2 | 2.01                     | 0.61              |
| 22:AV:3:C:H42      | 22:AV:70:G:H1     | 1.47                     | 0.61              |
| 22:AW:60:A:H2'     | 22:AW:61:U:H5'    | 1.81                     | 0.61              |
| 22:AW:75:C:H5'     | 22:AW:75:C:H6     | 1.66                     | 0.61              |
| 23:AX:17:U:O2'     | 23:AX:18:G:H5'    | 2.01                     | 0.61              |
| 24:AY:82:ILE:HD12  | 24:AY:101:LEU:CD2 | 2.31                     | 0.61              |
| 24:AY:215:LYS:HA   | 24:AY:218:GLU:HB3 | 1.82                     | 0.61              |
| 26:B1:73:LEU:CD2   | 26:B1:94:LEU:HD23 | 2.31                     | 0.61              |
| 35:BA:1525:G:H2'   | 35:BA:1526:G:C8   | 2.36                     | 0.61              |
| 35:BA:1993:U:H4'   | 39:BE:128:SER:OG  | 2.00                     | 0.61              |
| 35:BA:2151:G:O2'   | 35:BA:2152:G:H5'  | 2.01                     | 0.61              |
| 35:BA:2298:A:H62   | 35:BA:2318:G:H8   | 1.49                     | 0.61              |
| 35:BA:813:U:H2'    | 35:BA:814:C:H6    | 1.66                     | 0.61              |
| 41:BG:125:PHE:HB3  | 41:BG:166:ASP:HB3 | 1.82                     | 0.61              |
| 42:BH:41:MET:HG2   | 42:BH:43:VAL:HG13 | 1.83                     | 0.61              |
| 44:BK:103:GLN:O    | 44:BK:106:GLU:HG2 | 2.00                     | 0.61              |
| 48:BP:9:ASN:H      | 48:BP:10:PRO:HD2  | 1.65                     | 0.61              |
| 48:BP:30:THR:CG2   | 48:BP:31:ALA:H    | 2.07                     | 0.61              |
| 51:BS:67:ARG:HB3   | 51:BS:71:ARG:NH2  | 2.16                     | 0.61              |
| 52:BT:134:GLU:O    | 52:BT:135:ALA:HB2 | 2.00                     | 0.61              |
| 2:CB:220:ASP:O     | 2:CB:223:ILE:N    | 2.34                     | 0.61              |
| 4:CD:126:ILE:HG22  | 4:CD:127:THR:N    | 2.15                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:CD:30:LYS:C     | 4:CD:32:ALA:N      | 2.48                     | 0.61              |
| 12:CL:84:LEU:HD23 | 12:CL:101:VAL:HG21 | 1.82                     | 0.61              |
| 24:CY:315:LYS:HZ3 | 24:CY:317:MET:HG2  | 1.66                     | 0.61              |
| 31:D6:35:GLU:HA   | 31:D6:35:GLU:OE1   | 2.00                     | 0.61              |
| 34:D9:29:ASN:O    | 34:D9:29:ASN:ND2   | 2.33                     | 0.61              |
| 35:DA:11:G:H22    | 35:DA:2628:C:P     | 2.24                     | 0.61              |
| 35:DA:2009:G:H1'  | 50:DR:107:ASP:O    | 2.00                     | 0.61              |
| 35:DA:2186:G:C3'  | 35:DA:2187:G:H5''  | 2.31                     | 0.61              |
| 35:DA:2454:G:C2'  | 35:DA:2455:G:H5'   | 2.30                     | 0.61              |
| 35:DA:2774:C:H2'  | 35:DA:2775:A:O4'   | 2.00                     | 0.61              |
| 35:DA:30:G:O2'    | 35:DA:31:C:H5'     | 2.01                     | 0.61              |
| 35:DA:589:C:O2'   | 35:DA:590:A:H5'    | 2.01                     | 0.61              |
| 35:DA:811:U:O2'   | 35:DA:812:C:H5''   | 2.01                     | 0.61              |
| 35:DA:986:C:O2'   | 35:DA:987:G:H5'    | 2.01                     | 0.61              |
| 36:DB:91:C:O2'    | 36:DB:92:C:H5'     | 2.01                     | 0.61              |
| 38:DD:134:ARG:HG3 | 38:DD:135:PHE:CD1  | 2.36                     | 0.61              |
| 42:DH:44:VAL:O    | 42:DH:50:VAL:HG13  | 2.01                     | 0.61              |
| 46:DN:43:THR:HB   | 46:DN:46:VAL:HG11  | 1.82                     | 0.61              |
| 46:DN:46:VAL:O    | 46:DN:47:ALA:HB3   | 2.01                     | 0.61              |
| 48:DP:24:GLY:HA2  | 48:DP:33:ARG:NH1   | 2.16                     | 0.61              |
| 50:DR:117:VAL:CG1 | 50:DR:118:GLU:N    | 2.63                     | 0.61              |
| 1:CA:1432:G:OP1   | 52:DT:107:ASP:HB2  | 1.99                     | 0.61              |
| 30:D5:27:PRO:CG   | 55:DW:23:LEU:HD11  | 2.31                     | 0.61              |
| 1:AA:54:C:H2'     | 1:AA:352:C:H41     | 1.66                     | 0.61              |
| 1:AA:882:C:O2'    | 1:AA:883:C:H5'     | 2.00                     | 0.61              |
| 3:AC:110:ASN:OD1  | 3:AC:140:ARG:HD2   | 2.01                     | 0.61              |
| 3:AC:148:GLY:HA3  | 3:AC:172:ARG:O     | 2.01                     | 0.61              |
| 3:AC:99:VAL:HG23  | 3:AC:99:VAL:O      | 2.01                     | 0.61              |
| 1:AA:1226:C:N4    | 13:AM:104:ARG:HD2  | 2.16                     | 0.61              |
| 20:AT:36:LEU:HD12 | 20:AT:59:ALA:HB2   | 1.82                     | 0.61              |
| 22:AV:46:G:O3'    | 22:AV:47:U:C6      | 2.51                     | 0.61              |
| 24:AY:238:THR:CG2 | 24:AY:241:GLU:H    | 2.14                     | 0.61              |
| 24:AY:634:MET:HA  | 24:AY:642:VAL:O    | 2.01                     | 0.61              |
| 30:B5:20:ARG:HG2  | 30:B5:23:HIS:CD2   | 2.35                     | 0.61              |
| 30:B5:40:LYS:HZ3  | 30:B5:46:CYS:H     | 1.47                     | 0.61              |
| 35:BA:1297:C:H2'  | 35:BA:1298:C:H6    | 1.66                     | 0.61              |
| 35:BA:1516:C:H2'  | 35:BA:1517:G:C5'   | 2.30                     | 0.61              |
| 35:BA:1717:G:H2'  | 35:BA:1718:G:H5''  | 1.81                     | 0.61              |
| 35:BA:1775:U:C2'  | 35:BA:1776:G:H5'   | 2.31                     | 0.61              |
| 35:BA:2000:G:O2'  | 35:BA:2001:A:H5'   | 2.01                     | 0.61              |
| 26:B1:45:ASN:CB   | 35:BA:2230:G:H1'   | 2.28                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:2573:C:O2    | 35:BA:2573:C:H2'   | 2.00                     | 0.61              |
| 35:BA:364:C:H2'    | 35:BA:365:C:C5'    | 2.30                     | 0.61              |
| 35:BA:514:A:H2'    | 35:BA:515:A:C8     | 2.36                     | 0.61              |
| 35:BA:710:G:H1     | 35:BA:721:C:H42    | 1.47                     | 0.61              |
| 36:BB:112:U:H2'    | 36:BB:113:G:C8     | 2.34                     | 0.61              |
| 39:BE:44:TYR:O     | 39:BE:45:THR:HB    | 1.99                     | 0.61              |
| 41:BG:39:ILE:CG1   | 41:BG:92:VAL:HG22  | 2.30                     | 0.61              |
| 44:BK:3:LYS:HD3    | 44:BK:29:GLN:HG2   | 1.82                     | 0.61              |
| 47:BO:114:ILE:HD12 | 47:BO:114:ILE:N    | 2.14                     | 0.61              |
| 48:BP:84:ASN:C     | 48:BP:86:LYS:H     | 2.04                     | 0.61              |
| 54:BV:39:LEU:HD12  | 54:BV:50:PRO:O     | 2.01                     | 0.61              |
| 1:CA:1314:C:H2'    | 1:CA:1315:U:C6     | 2.36                     | 0.61              |
| 1:CA:1478:C:H2'    | 1:CA:1479:C:H6     | 1.64                     | 0.61              |
| 1:CA:505:G:H2'     | 1:CA:506:G:H8      | 1.66                     | 0.61              |
| 18:CR:37:VAL:CG2   | 18:CR:38:GLU:H     | 2.07                     | 0.61              |
| 24:CY:281:PRO:HB2  | 24:CY:286:ILE:CD1  | 2.31                     | 0.61              |
| 24:CY:341:VAL:HG23 | 24:CY:342:TYR:N    | 2.15                     | 0.61              |
| 24:CY:438:PHE:CD2  | 24:CY:438:PHE:C    | 2.74                     | 0.61              |
| 25:D0:43:THR:HG22  | 35:DA:2331:G:O3'   | 2.01                     | 0.61              |
| 31:D6:15:GLU:CB    | 31:D6:47:THR:HG21  | 2.31                     | 0.61              |
| 34:D9:1:MET:O      | 34:D9:34:GLN:HG2   | 2.01                     | 0.61              |
| 34:D9:22:ARG:HB2   | 34:D9:24:TYR:HE1   | 1.66                     | 0.61              |
| 35:DA:1105:U:H2'   | 35:DA:1106:G:O4'   | 2.00                     | 0.61              |
| 35:DA:2021:C:H4'   | 35:DA:2022:U:OP2   | 2.01                     | 0.61              |
| 35:DA:2069:G:O2'   | 35:DA:2070:G:H5'   | 2.01                     | 0.61              |
| 35:DA:2712:U:H1'   | 35:DA:2712(A):A:C8 | 2.36                     | 0.61              |
| 35:DA:537:C:H2'    | 35:DA:538:G:H8     | 1.65                     | 0.61              |
| 37:DC:71:LYS:HG2   | 37:DC:72:GLN:H     | 1.66                     | 0.61              |
| 52:DT:28:VAL:HG22  | 52:DT:47:GLY:N     | 2.16                     | 0.61              |
| 54:DV:2:PHE:O      | 54:DV:3:ALA:HB3    | 2.01                     | 0.61              |
| 57:DY:88:LYS:HZ3   | 57:DY:93:GLY:C     | 2.04                     | 0.61              |
| 1:AA:1314:C:H2'    | 1:AA:1315:U:C6     | 2.36                     | 0.60              |
| 1:AA:339:C:OP2     | 47:BO:97:ARG:NH1   | 2.34                     | 0.60              |
| 1:AA:487:A:H2'     | 1:AA:488:C:O4'     | 2.01                     | 0.60              |
| 1:AA:687:A:N6      | 1:AA:703:G:H1'     | 2.14                     | 0.60              |
| 7:AG:7:ALA:O       | 7:AG:8:GLU:HB2     | 1.99                     | 0.60              |
| 20:AT:45:GLN:HA    | 20:AT:91:LEU:HB3   | 1.82                     | 0.60              |
| 20:AT:50:GLU:HB3   | 20:AT:99:LEU:HB2   | 1.82                     | 0.60              |
| 24:AY:122:TRP:C    | 24:AY:124:GLN:H    | 2.03                     | 0.60              |
| 25:B0:42:GLY:HA3   | 35:BA:2331:G:O4'   | 2.00                     | 0.60              |
| 35:BA:1080:C:O2'   | 44:BK:126:MET:HG3  | 2.01                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:1493:C:C4    | 35:BA:2206:G:O2'   | 2.53                     | 0.60              |
| 35:BA:2312:U:OP1   | 41:BG:73:ALA:HA    | 2.00                     | 0.60              |
| 35:BA:321:G:C2     | 35:BA:341:G:H4'    | 2.36                     | 0.60              |
| 40:BF:63:LYS:HG3   | 40:BF:76:GLY:HA2   | 1.83                     | 0.60              |
| 40:BF:89:VAL:HG12  | 40:BF:90:PHE:H     | 1.66                     | 0.60              |
| 44:BK:78:ILE:HD11  | 44:BK:136:VAL:HG11 | 1.83                     | 0.60              |
| 46:BN:128:HIS:HE1  | 46:BN:134:ARG:HH11 | 1.47                     | 0.60              |
| 46:BN:134:ARG:O    | 46:BN:136:GLU:N    | 2.31                     | 0.60              |
| 48:BP:146:VAL:O    | 48:BP:148:LEU:N    | 2.34                     | 0.60              |
| 48:BP:24:GLY:HA2   | 48:BP:33:ARG:NH1   | 2.16                     | 0.60              |
| 49:BQ:60:ARG:HB2   | 49:BQ:60:ARG:NH1   | 2.16                     | 0.60              |
| 55:BW:95:ILE:O     | 55:BW:95:ILE:HG13  | 2.00                     | 0.60              |
| 57:BY:28:LYS:O     | 57:BY:38:ILE:HG22  | 2.00                     | 0.60              |
| 1:CA:1275:A:O2'    | 1:CA:1276:G:H5'    | 2.01                     | 0.60              |
| 1:CA:1425:U:O2'    | 1:CA:1426:C:H5'    | 2.01                     | 0.60              |
| 1:CA:390:C:H2'     | 1:CA:391:G:H8      | 1.66                     | 0.60              |
| 2:CB:32:ILE:HD11   | 2:CB:40:HIS:HB3    | 1.83                     | 0.60              |
| 4:CD:15:GLU:O      | 4:CD:17:VAL:HG23   | 2.00                     | 0.60              |
| 1:CA:390:C:O3'     | 16:CP:28:ARG:NH2   | 2.33                     | 0.60              |
| 18:CR:74:ARG:HD3   | 18:CR:81:PHE:CD2   | 2.36                     | 0.60              |
| 24:CY:153:MET:O    | 24:CY:157:LEU:HG   | 2.01                     | 0.60              |
| 26:D1:80:LEU:CD2   | 26:D1:81:LYS:H     | 2.14                     | 0.60              |
| 29:D4:9:LEU:CD2    | 41:DG:65:GLY:HA3   | 2.31                     | 0.60              |
| 35:DA:1833:U:H2'   | 35:DA:1834:U:H6    | 1.66                     | 0.60              |
| 35:DA:1885:A:H5'   | 35:DA:1885:A:H8    | 1.65                     | 0.60              |
| 35:DA:2151:G:O2'   | 35:DA:2152:G:H5'   | 2.01                     | 0.60              |
| 35:DA:2891:G:H4'   | 35:DA:2892:A:OP1   | 2.01                     | 0.60              |
| 36:DB:92:C:H2'     | 36:DB:93:G:H8      | 1.65                     | 0.60              |
| 35:DA:1658:C:OP1   | 39:DE:132:HIS:O    | 2.19                     | 0.60              |
| 40:DF:181:LEU:HB3  | 40:DF:205:ARG:HH11 | 1.65                     | 0.60              |
| 41:DG:107:LEU:HD11 | 41:DG:178:PHE:HE1  | 1.65                     | 0.60              |
| 42:DH:153:LYS:HG3  | 42:DH:154:PRO:CD   | 2.31                     | 0.60              |
| 42:DH:85:LYS:O     | 42:DH:85:LYS:HD3   | 2.01                     | 0.60              |
| 52:DT:10:VAL:O     | 52:DT:12:SER:N     | 2.34                     | 0.60              |
| 55:DW:95:ILE:O     | 55:DW:95:ILE:HG13  | 1.99                     | 0.60              |
| 1:AA:165:C:O2'     | 1:AA:166:G:H5'     | 2.01                     | 0.60              |
| 1:AA:41:G:H2'      | 1:AA:42:G:C8       | 2.36                     | 0.60              |
| 5:AE:78:HIS:O      | 5:AE:93:PRO:HD3    | 2.01                     | 0.60              |
| 11:AK:59:TYR:O     | 11:AK:62:GLN:HB3   | 2.01                     | 0.60              |
| 14:AN:16:PHE:N     | 14:AN:16:PHE:CD1   | 2.62                     | 0.60              |
| 22:AW:15:G:H21     | 22:AW:22:A:H1'     | 1.66                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 61:AY:702:FUA:H12  | 61:AY:702:FUA:O1    | 2.00                     | 0.60              |
| 31:B6:15:GLU:OE2   | 31:B6:20:ASN:ND2    | 2.33                     | 0.60              |
| 35:BA:1125:G:H3'   | 35:BA:1126:A:H5''   | 1.83                     | 0.60              |
| 35:BA:11:G:H2'     | 35:BA:12:U:C6       | 2.35                     | 0.60              |
| 35:BA:134:C:H2'    | 35:BA:135:G:H8      | 1.64                     | 0.60              |
| 35:BA:2056:G:H2'   | 35:BA:2056:G:N3     | 2.14                     | 0.60              |
| 35:BA:2262:U:C2'   | 35:BA:2263:C:H5''   | 2.32                     | 0.60              |
| 38:BD:148:GLU:HB2  | 38:BD:151:LYS:HG3   | 1.83                     | 0.60              |
| 38:BD:166:GLN:CA   | 38:BD:166:GLN:HE21  | 2.13                     | 0.60              |
| 52:BT:28:VAL:HG22  | 52:BT:47:GLY:H      | 1.66                     | 0.60              |
| 1:CA:1132:C:O2'    | 1:CA:1133:G:H5'     | 2.00                     | 0.60              |
| 3:CC:14:ILE:O      | 3:CC:15:THR:HB      | 2.01                     | 0.60              |
| 3:CC:94:LEU:O      | 3:CC:95:THR:HG23    | 2.01                     | 0.60              |
| 6:CF:38:GLU:O      | 6:CF:39:LYS:O       | 2.18                     | 0.60              |
| 13:CM:90:LEU:O     | 13:CM:91:ARG:C      | 2.40                     | 0.60              |
| 24:CY:187:THR:HG22 | 24:CY:197:ARG:O     | 2.01                     | 0.60              |
| 33:D8:30:ARG:O     | 33:D8:31:HIS:HB3    | 2.02                     | 0.60              |
| 35:DA:2259:G:O2'   | 35:DA:2260:C:H5'    | 2.01                     | 0.60              |
| 35:DA:2712:U:O2'   | 35:DA:2712(A):A:O5' | 2.19                     | 0.60              |
| 35:DA:481:G:H2'    | 35:DA:507:A:N1      | 2.16                     | 0.60              |
| 35:DA:605:C:H2'    | 35:DA:606:U:H6      | 1.66                     | 0.60              |
| 35:DA:622:G:O2'    | 35:DA:623:G:H5'     | 2.01                     | 0.60              |
| 35:DA:779:U:OP1    | 38:DD:49:ILE:HG23   | 2.00                     | 0.60              |
| 38:DD:76:PRO:HG2   | 38:DD:98:VAL:CG2    | 2.31                     | 0.60              |
| 40:DF:9:ILE:HG23   | 40:DF:13:SER:O      | 2.00                     | 0.60              |
| 40:DF:185:ASP:OD1  | 40:DF:188:ARG:HD3   | 2.01                     | 0.60              |
| 40:DF:63:LYS:HG3   | 40:DF:76:GLY:HA2    | 1.82                     | 0.60              |
| 46:DN:55:VAL:HG21  | 46:DN:127:ASP:N     | 2.16                     | 0.60              |
| 49:DQ:21:THR:HG23  | 49:DQ:101:ARG:HB2   | 1.82                     | 0.60              |
| 49:DQ:11:LYS:NZ    | 49:DQ:88:GLY:O      | 2.34                     | 0.60              |
| 52:DT:134:GLU:O    | 52:DT:135:ALA:HB2   | 1.99                     | 0.60              |
| 57:DY:88:LYS:NZ    | 57:DY:93:GLY:O      | 2.31                     | 0.60              |
| 1:AA:1117:G:H5'    | 1:AA:1117:G:H8      | 1.64                     | 0.60              |
| 1:AA:769:G:H4'     | 1:AA:1513:A:H4'     | 1.82                     | 0.60              |
| 9:AI:3:GLN:NE2     | 9:AI:20:ARG:HH21    | 1.99                     | 0.60              |
| 35:BA:1049:C:H2'   | 35:BA:1050:A:H8     | 1.66                     | 0.60              |
| 35:BA:1380:G:H2'   | 35:BA:1381:G:H8     | 1.65                     | 0.60              |
| 35:BA:92:A:H2'     | 35:BA:93:G:C8       | 2.36                     | 0.60              |
| 35:BA:990:A:N6     | 35:BA:1186:G:H1'    | 2.16                     | 0.60              |
| 39:BE:98:PRO:HG3   | 39:BE:175:VAL:HG12  | 1.82                     | 0.60              |
| 35:BA:797:C:OP1    | 40:BF:62:ARG:HG3    | 2.01                     | 0.60              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:BK:14:ALA:HA    | 44:BK:41:PHE:CZ    | 2.36                     | 0.60              |
| 46:BN:67:LEU:HB3   | 46:BN:88:GLU:HG3   | 1.81                     | 0.60              |
| 50:BR:12:ARG:HG3   | 50:BR:12:ARG:HH11  | 1.66                     | 0.60              |
| 52:BT:30:VAL:HG21  | 52:BT:83:ILE:HG12  | 1.83                     | 0.60              |
| 52:BT:50:ILE:HD12  | 52:BT:50:ILE:N     | 2.16                     | 0.60              |
| 1:CA:1016:A:H2'    | 1:CA:1017:G:O4'    | 2.02                     | 0.60              |
| 1:CA:1303:C:C2'    | 1:CA:1304:G:H5'    | 2.31                     | 0.60              |
| 1:CA:925:G:H5'     | 1:CA:926:G:OP1     | 2.01                     | 0.60              |
| 2:CB:155:LEU:HD13  | 2:CB:155:LEU:C     | 2.21                     | 0.60              |
| 4:CD:18:LYS:C      | 4:CD:19:LEU:HD12   | 2.22                     | 0.60              |
| 12:CL:41:ARG:NH1   | 12:CL:41:ARG:HB3   | 2.13                     | 0.60              |
| 20:CT:36:LEU:HD12  | 20:CT:59:ALA:HB2   | 1.82                     | 0.60              |
| 22:CW:68:C:H2'     | 22:CW:69:C:C6      | 2.37                     | 0.60              |
| 24:CY:28:THR:O     | 24:CY:32:ILE:HG13  | 2.01                     | 0.60              |
| 24:CY:308:PRO:O    | 24:CY:332:SER:HB2  | 2.02                     | 0.60              |
| 26:D1:41:ARG:NH2   | 35:DA:1365:A:H5'   | 2.16                     | 0.60              |
| 33:D8:51:ALA:C     | 33:D8:53:PRO:HD2   | 2.22                     | 0.60              |
| 35:DA:1231:G:H2'   | 35:DA:1232:G:H8    | 1.65                     | 0.60              |
| 35:DA:1290:C:H2'   | 35:DA:1291:C:C6    | 2.37                     | 0.60              |
| 35:DA:2040:C:H2'   | 35:DA:2041:U:H6    | 1.67                     | 0.60              |
| 35:DA:2240:C:O2'   | 35:DA:2241:A:H5'   | 2.02                     | 0.60              |
| 35:DA:2462:U:H2'   | 35:DA:2463:C:H6    | 1.66                     | 0.60              |
| 35:DA:2762:G:H8    | 35:DA:2762:G:H5'   | 1.67                     | 0.60              |
| 26:D1:25:LYS:HB2   | 35:DA:388:G:H5'    | 1.83                     | 0.60              |
| 40:DF:154:VAL:HG13 | 40:DF:191:ARG:O    | 2.01                     | 0.60              |
| 40:DF:28:ILE:O     | 40:DF:30:PRO:HD3   | 2.01                     | 0.60              |
| 41:DG:110:ALA:CB   | 41:DG:140:ILE:HD13 | 2.32                     | 0.60              |
| 41:DG:122:PRO:HG2  | 41:DG:123:ASN:OD1  | 2.01                     | 0.60              |
| 42:DH:28:GLY:HA3   | 42:DH:79:VAL:CG2   | 2.31                     | 0.60              |
| 46:DN:65:LYS:HA    | 46:DN:65:LYS:HZ3   | 1.67                     | 0.60              |
| 47:DO:87:ILE:HD13  | 47:DO:87:ILE:N     | 2.16                     | 0.60              |
| 48:DP:124:LYS:HD3  | 48:DP:143:GLY:HA3  | 1.81                     | 0.60              |
| 50:DR:28:LEU:C     | 50:DR:28:LEU:HD23  | 2.21                     | 0.60              |
| 52:DT:57:PHE:C     | 52:DT:58:ASN:HD22  | 2.04                     | 0.60              |
| 1:AA:1303:C:H2'    | 1:AA:1304:G:H5'    | 1.84                     | 0.60              |
| 1:AA:72:C:H2'      | 1:AA:73:G:C8       | 2.37                     | 0.60              |
| 2:AB:156:LYS:O     | 2:AB:157:ARG:HB3   | 2.01                     | 0.60              |
| 5:AE:20:GLN:O      | 5:AE:21:ALA:C      | 2.39                     | 0.60              |
| 6:AF:16:GLN:CD     | 6:AF:16:GLN:H      | 2.03                     | 0.60              |
| 17:AQ:76:LEU:HD12  | 17:AQ:77:VAL:N     | 2.16                     | 0.60              |
| 18:AR:58:LEU:HD12  | 18:AR:58:LEU:N     | 2.17                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:AT:93:GLU:C     | 20:AT:95:ALA:H     | 2.02                     | 0.60              |
| 24:AY:180:VAL:HG23 | 24:AY:181:LEU:N    | 2.17                     | 0.60              |
| 24:AY:512:ILE:H    | 24:AY:512:ILE:CD1  | 2.14                     | 0.60              |
| 31:B6:45:LYS:HE3   | 35:BA:2371:G:H5''  | 1.83                     | 0.60              |
| 35:BA:1467:C:H5    | 35:BA:1546:C:H2'   | 1.66                     | 0.60              |
| 35:BA:2787:C:H1'   | 39:BE:61:ARG:CG    | 2.30                     | 0.60              |
| 35:BA:693:C:O2'    | 35:BA:694:U:H5'    | 2.01                     | 0.60              |
| 35:BA:723:G:H2'    | 35:BA:724:U:C6     | 2.36                     | 0.60              |
| 37:BC:213:VAL:HG12 | 37:BC:225:ILE:HD11 | 1.82                     | 0.60              |
| 39:BE:170:LEU:N    | 39:BE:170:LEU:HD12 | 2.16                     | 0.60              |
| 40:BF:157:VAL:HG22 | 40:BF:194:MET:HG2  | 1.83                     | 0.60              |
| 42:BH:156:ALA:O    | 42:BH:158:HIS:HD2  | 1.84                     | 0.60              |
| 46:BN:22:THR:HA    | 46:BN:61:ARG:O     | 2.00                     | 0.60              |
| 49:BQ:66:ILE:HG13  | 49:BQ:66:ILE:O     | 2.01                     | 0.60              |
| 30:B5:55:ARG:HH12  | 50:BR:33:ARG:HD2   | 1.66                     | 0.60              |
| 47:BO:104:ARG:NE   | 52:BT:33:LYS:HE3   | 2.14                     | 0.60              |
| 53:BU:55:ARG:HA    | 53:BU:58:ARG:HG3   | 1.82                     | 0.60              |
| 53:BU:83:LEU:HD12  | 53:BU:83:LEU:N     | 2.16                     | 0.60              |
| 54:BV:2:PHE:O      | 54:BV:3:ALA:HB3    | 2.01                     | 0.60              |
| 58:BZ:108:PRO:HG2  | 58:BZ:111:VAL:HG23 | 1.82                     | 0.60              |
| 1:CA:1101:A:H4'    | 1:CA:1102:A:C4'    | 2.32                     | 0.60              |
| 1:CA:1254:C:H2'    | 1:CA:1255:G:C8     | 2.36                     | 0.60              |
| 1:CA:1479:C:H2'    | 1:CA:1480:G:H8     | 1.67                     | 0.60              |
| 8:CH:6:ILE:HD12    | 8:CH:6:ILE:N       | 2.16                     | 0.60              |
| 19:CS:14:HIS:CD2   | 19:CS:15:LEU:HD23  | 2.33                     | 0.60              |
| 24:CY:185:ALA:HB3  | 24:CY:199:ILE:O    | 2.01                     | 0.60              |
| 31:D6:15:GLU:OE2   | 31:D6:20:ASN:ND2   | 2.34                     | 0.60              |
| 35:DA:1075:C:H5'   | 35:DA:1076:C:OP2   | 2.01                     | 0.60              |
| 35:DA:279:C:H3'    | 35:DA:280:C:H5''   | 1.82                     | 0.60              |
| 35:DA:518:G:H4'    | 55:DW:18:ARG:NH1   | 2.15                     | 0.60              |
| 35:DA:892:G:H2'    | 35:DA:893:C:C6     | 2.36                     | 0.60              |
| 37:DC:128:LEU:HD11 | 37:DC:132:LEU:HG   | 1.83                     | 0.60              |
| 38:DD:31:LYS:NZ    | 38:DD:33:LEU:HB2   | 2.16                     | 0.60              |
| 41:DG:61:ALA:HA    | 41:DG:64:THR:HG22  | 1.83                     | 0.60              |
| 52:DT:25:GLY:HA2   | 52:DT:92:GLY:CA    | 2.32                     | 0.60              |
| 54:DV:1:MET:HE2    | 54:DV:1:MET:HA     | 1.82                     | 0.60              |
| 57:DY:44:ILE:HG22  | 57:DY:45:VAL:N     | 2.16                     | 0.60              |
| 58:DZ:158:PRO:HD2  | 58:DZ:161:VAL:HG21 | 1.82                     | 0.60              |
| 1:AA:1053:G:C3'    | 1:AA:1054:C:H5'    | 2.31                     | 0.60              |
| 1:AA:1137:C:H4'    | 1:AA:1138:G:C2     | 2.36                     | 0.60              |
| 1:AA:201:C:H2'     | 1:AA:202:U:H5''    | 1.83                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:22:G:O2'      | 1:AA:23:C:H5'      | 2.01                     | 0.60              |
| 5:AE:15:ARG:HG3    | 5:AE:28:PHE:CE2    | 2.37                     | 0.60              |
| 6:AF:33:TYR:HA     | 6:AF:71:ARG:NH2    | 2.16                     | 0.60              |
| 10:AJ:3:LYS:NZ     | 10:AJ:76:ASN:HA    | 2.16                     | 0.60              |
| 31:B6:15:GLU:CD    | 31:B6:44:ARG:HH12  | 2.05                     | 0.60              |
| 35:BA:1094:U:H2'   | 35:BA:1096:A:OP2   | 2.00                     | 0.60              |
| 35:BA:1022:G:N2    | 35:BA:1142(A):A:H2 | 1.99                     | 0.60              |
| 35:BA:1682:G:H2'   | 35:BA:1683:C:H6    | 1.64                     | 0.60              |
| 35:BA:175:G:O2'    | 35:BA:176:G:H5'    | 2.02                     | 0.60              |
| 35:BA:2040:C:H2'   | 35:BA:2041:U:C6    | 2.36                     | 0.60              |
| 35:BA:510:C:H3'    | 35:BA:510:C:OP1    | 2.01                     | 0.60              |
| 35:BA:848:G:O6     | 35:BA:928:G:H2'    | 2.01                     | 0.60              |
| 37:BC:65:LEU:HD13  | 37:BC:189:ASN:ND2  | 2.16                     | 0.60              |
| 38:BD:155:LEU:N    | 38:BD:155:LEU:HD12 | 2.16                     | 0.60              |
| 40:BF:181:LEU:HB3  | 40:BF:205:ARG:HH11 | 1.64                     | 0.60              |
| 40:BF:53:THR:CG2   | 40:BF:56:GLU:HG3   | 2.17                     | 0.60              |
| 52:BT:98:LYS:HB3   | 52:BT:100:TYR:HE1  | 1.66                     | 0.60              |
| 56:BX:10:ALA:O     | 56:BX:28:PHE:HB2   | 2.00                     | 0.60              |
| 35:BA:481:G:OP2    | 57:BY:47:LYS:HD3   | 2.01                     | 0.60              |
| 58:BZ:63:ASP:HB2   | 58:BZ:65:GLN:HE21  | 1.66                     | 0.60              |
| 1:CA:1348:U:H2'    | 1:CA:1349:A:H8     | 1.67                     | 0.60              |
| 2:CB:172:ILE:HD12  | 2:CB:172:ILE:N     | 2.12                     | 0.60              |
| 3:CC:133:ALA:O     | 3:CC:137:ALA:HB2   | 2.02                     | 0.60              |
| 6:CF:42:GLU:O      | 6:CF:44:GLY:N      | 2.34                     | 0.60              |
| 12:CL:117:ARG:NH2  | 12:CL:124:LYS:HB2  | 2.17                     | 0.60              |
| 24:CY:415:PRO:HA   | 24:CY:474:ALA:CB   | 2.32                     | 0.60              |
| 24:CY:489:LYS:CG   | 24:CY:598:ASP:HB2  | 2.31                     | 0.60              |
| 33:D8:33:ASN:N     | 33:D8:36:LYS:HD2   | 2.16                     | 0.60              |
| 35:DA:1168:G:H2'   | 35:DA:1169:G:C8    | 2.37                     | 0.60              |
| 35:DA:1971:A:C4    | 38:DD:241:PRO:HD3  | 2.37                     | 0.60              |
| 35:DA:2377:A:H2'   | 35:DA:2378:A:C8    | 2.36                     | 0.60              |
| 35:DA:2572:A:H5'   | 35:DA:2574:G:C4'   | 2.29                     | 0.60              |
| 35:DA:363(A):A:H2' | 35:DA:363(B):G:H8  | 1.67                     | 0.60              |
| 39:DE:179:GLU:HB3  | 39:DE:181:LEU:CD2  | 2.31                     | 0.60              |
| 40:DF:185:ASP:HA   | 40:DF:188:ARG:HG2  | 1.83                     | 0.60              |
| 40:DF:18:ARG:HG2   | 40:DF:19:GLU:H     | 1.67                     | 0.60              |
| 41:DG:112:PRO:C    | 41:DG:113:ARG:HA   | 2.21                     | 0.60              |
| 41:DG:120:LEU:HD12 | 41:DG:180:PHE:HE2  | 1.66                     | 0.60              |
| 44:DK:79:ARG:HD2   | 44:DK:85:GLU:O     | 2.00                     | 0.60              |
| 47:DO:47:ILE:HG22  | 47:DO:48:PRO:HD2   | 1.83                     | 0.60              |
| 48:DP:23:PRO:HB2   | 48:DP:33:ARG:NE    | 2.16                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 52:DT:29:ARG:HD3   | 52:DT:86:ILE:HG22 | 1.82                     | 0.60              |
| 53:DU:80:ILE:O     | 53:DU:84:LYS:HB2  | 2.02                     | 0.60              |
| 58:DZ:150:LEU:HD23 | 58:DZ:150:LEU:N   | 2.15                     | 0.60              |
| 1:AA:45:U:H2'      | 1:AA:46:G:H8      | 1.66                     | 0.60              |
| 9:AI:53:VAL:HG23   | 9:AI:55:ALA:HB3   | 1.82                     | 0.60              |
| 10:AJ:55:LYS:N     | 10:AJ:55:LYS:CE   | 2.62                     | 0.60              |
| 10:AJ:34:VAL:CG2   | 10:AJ:74:ILE:HG22 | 2.23                     | 0.60              |
| 12:AL:47:LYS:HB3   | 12:AL:48:PRO:HD3  | 1.83                     | 0.60              |
| 26:B1:90:ILE:O     | 26:B1:94:LEU:HD12 | 2.01                     | 0.60              |
| 33:B8:51:ALA:N     | 33:B8:53:PRO:HD2  | 2.17                     | 0.60              |
| 35:BA:1649:G:O2'   | 35:BA:1650:G:H5'  | 2.02                     | 0.60              |
| 35:BA:214:G:H1'    | 35:BA:216:A:O2'   | 2.01                     | 0.60              |
| 35:BA:2186:G:C3'   | 35:BA:2187:G:H5'' | 2.31                     | 0.60              |
| 35:BA:198:C:H42    | 35:BA:248:G:H1    | 1.49                     | 0.60              |
| 35:BA:748:G:O6     | 35:BA:751:A:H4'   | 2.02                     | 0.60              |
| 41:BG:99:MET:O     | 41:BG:102:PHE:HB3 | 2.00                     | 0.60              |
| 41:BG:34:LEU:HB2   | 41:BG:99:MET:CE   | 2.31                     | 0.60              |
| 48:BP:96:THR:HG22  | 48:BP:126:VAL:HB  | 1.84                     | 0.60              |
| 49:BQ:52:VAL:O     | 49:BQ:55:VAL:HG12 | 2.01                     | 0.60              |
| 49:BQ:2:LEU:HG     | 49:BQ:69:PHE:HE1  | 1.66                     | 0.60              |
| 50:BR:28:LEU:CD2   | 50:BR:29:LEU:HD12 | 2.31                     | 0.60              |
| 52:BT:65:LYS:CE    | 52:BT:66:VAL:H    | 2.05                     | 0.60              |
| 58:BZ:69:THR:HG22  | 58:BZ:90:VAL:CA   | 2.23                     | 0.60              |
| 1:CA:449:C:O2      | 16:CP:42:ARG:HD2  | 2.01                     | 0.60              |
| 1:CA:539:A:H2'     | 1:CA:540:G:C8     | 2.36                     | 0.60              |
| 2:CB:233:SER:CB    | 2:CB:234:PRO:CD   | 2.80                     | 0.60              |
| 3:CC:25:GLY:C      | 3:CC:27:LYS:H     | 2.05                     | 0.60              |
| 4:CD:107:ARG:HH21  | 4:CD:194:LEU:CD1  | 2.14                     | 0.60              |
| 6:CF:60:PHE:O      | 6:CF:61:LEU:HD12  | 2.02                     | 0.60              |
| 6:CF:8:ILE:HG23    | 6:CF:85:VAL:HG13  | 1.82                     | 0.60              |
| 13:CM:68:GLY:H     | 13:CM:71:ARG:CB   | 2.14                     | 0.60              |
| 17:CQ:57:VAL:HG23  | 17:CQ:58:GLU:N    | 2.16                     | 0.60              |
| 18:CR:45:SER:H     | 18:CR:51:LEU:HG   | 1.65                     | 0.60              |
| 24:CY:439:ARG:H    | 24:CY:452:SER:HB3 | 1.67                     | 0.60              |
| 26:D1:86:SER:HA    | 26:D1:89:GLU:OE2  | 2.01                     | 0.60              |
| 31:D6:30:THR:HG22  | 31:D6:32:ASN:ND2  | 2.16                     | 0.60              |
| 35:DA:1328:G:H8    | 35:DA:1328:G:O5'  | 1.84                     | 0.60              |
| 35:DA:1504:C:C3'   | 35:DA:1505:C:H5'' | 2.32                     | 0.60              |
| 35:DA:1677:A:H2'   | 35:DA:1678:G:C8   | 2.37                     | 0.60              |
| 35:DA:389:G:O4'    | 35:DA:2413:G:H4'  | 2.02                     | 0.60              |
| 35:DA:26:G:H1'     | 35:DA:515:A:H61   | 1.65                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:DA:786:C:O2'    | 35:DA:787:U:H5'   | 2.02                     | 0.60              |
| 35:DA:92:A:H2'     | 35:DA:93:G:C8     | 2.37                     | 0.60              |
| 41:DG:94:LEU:HD22  | 41:DG:98:ARG:HB3  | 1.83                     | 0.60              |
| 42:DH:124:GLU:HG3  | 42:DH:132:ARG:HG3 | 1.83                     | 0.60              |
| 48:DP:24:GLY:CA    | 48:DP:33:ARG:NH1  | 2.65                     | 0.60              |
| 30:D5:27:PRO:HG3   | 55:DW:23:LEU:CD1  | 2.30                     | 0.60              |
| 1:AA:1017:G:H2'    | 1:AA:1018:C:C6    | 2.37                     | 0.60              |
| 1:AA:1239:A:H62    | 1:AA:1299:A:N6    | 1.99                     | 0.60              |
| 1:AA:1490:C:C6     | 1:AA:1490:C:H5'   | 2.37                     | 0.60              |
| 2:AB:60:ASP:O      | 2:AB:64:ARG:NH2   | 2.35                     | 0.60              |
| 3:AC:154:SER:O     | 3:AC:165:THR:HA   | 2.02                     | 0.60              |
| 4:AD:92:VAL:O      | 4:AD:96:LEU:HD22  | 2.01                     | 0.60              |
| 13:AM:11:ARG:O     | 13:AM:13:LYS:N    | 2.35                     | 0.60              |
| 22:AW:28:U:H2'     | 22:AW:29:C:C6     | 2.36                     | 0.60              |
| 34:B9:29:ASN:ND2   | 34:B9:29:ASN:O    | 2.34                     | 0.60              |
| 35:BA:1516:C:H2'   | 35:BA:1517:G:H5'  | 1.84                     | 0.60              |
| 35:BA:1827:C:C2'   | 35:BA:1828:G:H5'  | 2.31                     | 0.60              |
| 35:BA:2552:U:O2    | 35:BA:2554:U:H5'  | 2.02                     | 0.60              |
| 35:BA:406:G:O2'    | 35:BA:407:G:H8    | 1.83                     | 0.60              |
| 37:BC:132:LEU:HB3  | 37:BC:138:LEU:N   | 2.17                     | 0.60              |
| 47:BO:26:LYS:HB3   | 47:BO:30:ALA:HB2  | 1.83                     | 0.60              |
| 48:BP:16:ARG:HH11  | 48:BP:16:ARG:HB2  | 1.65                     | 0.60              |
| 1:CA:1017:G:H2'    | 1:CA:1018:C:C6    | 2.37                     | 0.60              |
| 1:CA:1250:A:H2'    | 1:CA:1251:A:C8    | 2.36                     | 0.60              |
| 1:CA:677:U:H3      | 1:CA:713:G:H22    | 1.49                     | 0.60              |
| 10:CJ:4:ILE:HB     | 10:CJ:74:ILE:HD11 | 1.83                     | 0.60              |
| 14:CN:14:PRO:O     | 14:CN:15:LYS:O    | 2.20                     | 0.60              |
| 16:CP:21:VAL:HG11  | 16:CP:59:TRP:NE1  | 2.17                     | 0.60              |
| 18:CR:37:VAL:O     | 18:CR:39:VAL:N    | 2.33                     | 0.60              |
| 24:CY:459:LEU:HD12 | 24:CY:460:GLU:N   | 2.17                     | 0.60              |
| 35:DA:1467:C:H5    | 35:DA:1546:C:H2'  | 1.65                     | 0.60              |
| 35:DA:212:G:H5'    | 35:DA:212:G:C8    | 2.33                     | 0.60              |
| 35:DA:2299:G:O2'   | 35:DA:2300:G:H5'  | 2.02                     | 0.60              |
| 36:DB:106:G:H2'    | 36:DB:107:G:H8    | 1.67                     | 0.60              |
| 40:DF:185:ASP:HA   | 40:DF:188:ARG:CG  | 2.31                     | 0.60              |
| 41:DG:43:LEU:HD22  | 41:DG:43:LEU:N    | 2.17                     | 0.60              |
| 42:DH:171:LEU:CD2  | 42:DH:172:LYS:O   | 2.50                     | 0.60              |
| 46:DN:14:VAL:HG11  | 46:DN:137:LYS:HD2 | 1.82                     | 0.60              |
| 51:DS:89:ARG:HG3   | 51:DS:92:TYR:CB   | 2.31                     | 0.60              |
| 52:DT:90:GLN:HG2   | 52:DT:120:ARG:NH2 | 2.16                     | 0.60              |
| 53:DU:92:ARG:NH1   | 54:DV:11:GLN:HG3  | 2.16                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 54:DV:39:LEU:HD12  | 54:DV:50:PRO:O     | 2.02                     | 0.60              |
| 1:AA:1510:U:H2'    | 1:AA:1511:G:H8     | 1.65                     | 0.60              |
| 1:AA:189:G:H2'     | 1:AA:189(A):C:C6   | 2.36                     | 0.60              |
| 1:AA:505:G:H2'     | 1:AA:506:G:H8      | 1.66                     | 0.60              |
| 1:AA:60:A:H5''     | 1:AA:331:G:N2      | 2.16                     | 0.60              |
| 7:AG:64:GLN:O      | 7:AG:67:GLU:HB3    | 2.02                     | 0.60              |
| 8:AH:89:PRO:HA     | 8:AH:92:ARG:HH11   | 1.66                     | 0.60              |
| 10:AJ:32:ALA:HB3   | 10:AJ:76:ASN:O     | 2.02                     | 0.60              |
| 24:AY:215:LYS:O    | 24:AY:219:VAL:N    | 2.34                     | 0.60              |
| 24:AY:248:LYS:O    | 24:AY:248:LYS:HG2  | 2.02                     | 0.60              |
| 24:AY:605:ILE:HG23 | 24:AY:646:PHE:HB3  | 1.82                     | 0.60              |
| 26:B1:6:GLU:OE1    | 26:B1:60:PHE:HA    | 2.02                     | 0.60              |
| 35:BA:1105:U:H2'   | 35:BA:1106:G:O4'   | 2.01                     | 0.60              |
| 35:BA:144:C:H2'    | 35:BA:145:G:C8     | 2.37                     | 0.60              |
| 35:BA:296:C:O2'    | 35:BA:297:C:H5'    | 2.02                     | 0.60              |
| 36:BB:48:A:H2'     | 36:BB:49:C:C6      | 2.37                     | 0.60              |
| 39:BE:179:GLU:HB3  | 39:BE:181:LEU:CD2  | 2.31                     | 0.60              |
| 35:BA:1245:G:H5''  | 40:BF:34:TRP:HZ2   | 1.66                     | 0.60              |
| 42:BH:105:LEU:CD2  | 42:BH:113:VAL:HB   | 2.32                     | 0.60              |
| 46:BN:57:ALA:N     | 46:BN:124:ALA:HA   | 2.16                     | 0.60              |
| 49:BQ:56:ARG:HH21  | 58:BZ:180:VAL:CG2  | 2.12                     | 0.60              |
| 25:B0:5:LYS:HB2    | 49:BQ:80:GLU:O     | 2.02                     | 0.60              |
| 52:BT:51:ARG:HG3   | 52:BT:98:LYS:HE3   | 1.84                     | 0.60              |
| 57:BY:105:ALA:C    | 57:BY:107:ASP:H    | 2.04                     | 0.60              |
| 1:CA:1053:G:C3'    | 1:CA:1054:C:H5'    | 2.31                     | 0.60              |
| 1:CA:1320:C:OP1    | 19:CS:70:LYS:NZ    | 2.35                     | 0.60              |
| 1:CA:723:U:H5'     | 1:CA:724:G:OP2     | 2.01                     | 0.60              |
| 1:CA:22:G:O2'      | 1:CA:913:A:N1      | 2.29                     | 0.60              |
| 2:CB:12:GLU:HA     | 2:CB:16:HIS:ND1    | 2.16                     | 0.60              |
| 7:CG:27:ILE:HD11   | 7:CG:40:ALA:HA     | 1.84                     | 0.60              |
| 9:CI:53:VAL:HG23   | 9:CI:55:ALA:HB3    | 1.83                     | 0.60              |
| 24:CY:377:VAL:HG21 | 24:CY:380:LEU:HD13 | 1.83                     | 0.60              |
| 25:D0:24:LYS:O     | 25:D0:25:ARG:HD3   | 2.01                     | 0.60              |
| 26:D1:60:PHE:CE1   | 26:D1:91:LYS:HE3   | 2.36                     | 0.60              |
| 28:D3:11:SER:HB3   | 35:DA:988:A:P      | 2.42                     | 0.60              |
| 35:DA:1125:G:H3'   | 35:DA:1126:A:H5''  | 1.84                     | 0.60              |
| 35:DA:1297:C:H2'   | 35:DA:1298:C:H6    | 1.66                     | 0.60              |
| 35:DA:144:C:H2'    | 35:DA:145:G:C8     | 2.36                     | 0.60              |
| 35:DA:552:G:H8     | 35:DA:552:G:H5'    | 1.67                     | 0.60              |
| 38:DD:71:ASP:CB    | 38:DD:103:ARG:HH22 | 2.04                     | 0.60              |
| 38:DD:145:VAL:HG22 | 38:DD:191:ALA:CB   | 2.31                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:DD:23:GLU:HA    | 38:DD:23:GLU:OE1   | 2.02                     | 0.60              |
| 40:DF:84:VAL:O     | 40:DF:86:GLY:N     | 2.32                     | 0.60              |
| 48:DP:146:VAL:HG22 | 48:DP:147:LEU:N    | 2.11                     | 0.60              |
| 52:DT:98:LYS:HB3   | 52:DT:100:TYR:HE1  | 1.67                     | 0.60              |
| 54:DV:32:THR:HG23  | 54:DV:59:ALA:O     | 2.01                     | 0.60              |
| 1:AA:1119:C:O2'    | 1:AA:1120:G:H5'    | 2.01                     | 0.60              |
| 1:AA:1323:G:H2'    | 1:AA:1324:A:H8     | 1.63                     | 0.60              |
| 1:AA:161:A:H2'     | 1:AA:162:A:H8      | 1.67                     | 0.60              |
| 12:AL:117:ARG:NH2  | 12:AL:124:LYS:HB2  | 2.17                     | 0.60              |
| 12:AL:34:ARG:HG3   | 12:AL:105:TYR:CE1  | 2.35                     | 0.60              |
| 24:AY:176:GLY:CA   | 24:AY:187:THR:HA   | 2.32                     | 0.60              |
| 24:AY:389:LEU:HD12 | 24:AY:389:LEU:N    | 2.16                     | 0.60              |
| 27:B2:36:ARG:HA    | 27:B2:39:ALA:HB3   | 1.82                     | 0.60              |
| 35:BA:143:G:H4'    | 56:BX:35:THR:HG21  | 1.84                     | 0.60              |
| 35:BA:1847:A:H3'   | 35:BA:1848:A:H5'   | 1.82                     | 0.60              |
| 35:BA:2175:C:H1'   | 37:BC:218:THR:O    | 2.02                     | 0.60              |
| 35:BA:2202:C:H2'   | 38:BD:151:LYS:NZ   | 2.16                     | 0.60              |
| 35:BA:2240:C:O2'   | 35:BA:2241:A:H5'   | 2.02                     | 0.60              |
| 35:BA:271(U):G:O2' | 35:BA:271(V):G:H5' | 2.01                     | 0.60              |
| 35:BA:259:G:H21    | 35:BA:621:A:H8     | 1.50                     | 0.60              |
| 44:BK:112:MET:HG3  | 44:BK:113:PRO:HD3  | 1.84                     | 0.60              |
| 35:BA:143(A):C:H4' | 56:BX:38:GLU:OE1   | 2.01                     | 0.60              |
| 1:CA:129(A):G:H5'' | 1:CA:129(A):G:H8   | 1.65                     | 0.60              |
| 1:CA:1356:G:H2'    | 1:CA:1357:A:H8     | 1.66                     | 0.60              |
| 1:CA:1479:C:O2'    | 1:CA:1480:G:H5'    | 2.02                     | 0.60              |
| 1:CA:445:G:H2'     | 1:CA:446:G:H8      | 1.66                     | 0.60              |
| 1:CA:861:G:O2'     | 1:CA:862:C:H5'     | 2.02                     | 0.60              |
| 3:CC:178:LEU:O     | 3:CC:180:ALA:N     | 2.34                     | 0.60              |
| 4:CD:131:ARG:HD3   | 4:CD:131:ARG:H     | 1.66                     | 0.60              |
| 6:CF:16:GLN:H      | 6:CF:16:GLN:CD     | 2.04                     | 0.60              |
| 9:CI:82:ALA:HA     | 9:CI:85:LEU:HD11   | 1.83                     | 0.60              |
| 19:CS:46:GLY:N     | 19:CS:62:ILE:HG23  | 2.16                     | 0.60              |
| 24:CY:276:VAL:HA   | 24:CY:280:LEU:HD23 | 1.82                     | 0.60              |
| 24:CY:609:GLU:H    | 24:CY:670:VAL:HG22 | 1.67                     | 0.60              |
| 24:CY:636:PRO:HB3  | 24:CY:641:GLN:OE1  | 2.02                     | 0.60              |
| 25:D0:36:ILE:O     | 25:D0:36:ILE:HG13  | 2.02                     | 0.60              |
| 31:D6:10:LEU:H     | 31:D6:10:LEU:HD22  | 1.64                     | 0.60              |
| 31:D6:11:LEU:HD22  | 31:D6:12:GLU:N     | 2.17                     | 0.60              |
| 31:D6:48:VAL:O     | 31:D6:49:HIS:HB2   | 2.02                     | 0.60              |
| 35:DA:1657:C:O2'   | 35:DA:1658:C:H5'   | 2.01                     | 0.60              |
| 35:DA:2450:A:O2'   | 35:DA:2451:A:H5'   | 2.01                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 35:DA:2472:G:H3'   | 35:DA:2475:C:N4     | 2.17                     | 0.60              |
| 35:DA:2794:C:H42   | 35:DA:2801(A):A:H61 | 1.50                     | 0.60              |
| 35:DA:78:A:O2'     | 35:DA:79:G:H5'      | 2.02                     | 0.60              |
| 38:DD:153:ALA:C    | 38:DD:154:LYS:HG3   | 2.21                     | 0.60              |
| 35:DA:322:A:H3'    | 40:DF:169:ASN:HD21  | 1.66                     | 0.60              |
| 40:DF:28:ILE:CD1   | 40:DF:28:ILE:H      | 2.15                     | 0.60              |
| 44:DK:14:ALA:HA    | 44:DK:41:PHE:CZ     | 2.37                     | 0.60              |
| 46:DN:35:ARG:O     | 46:DN:36:GLY:C      | 2.39                     | 0.60              |
| 47:DO:60:ALA:HA    | 47:DO:87:ILE:CD1    | 2.32                     | 0.60              |
| 48:DP:23:PRO:CB    | 48:DP:33:ARG:HG3    | 2.32                     | 0.60              |
| 51:DS:34:HIS:NE2   | 51:DS:54:LEU:HB3    | 2.16                     | 0.60              |
| 52:DT:83:ILE:HG13  | 52:DT:84:GLN:HG2    | 1.83                     | 0.60              |
| 1:AA:1005:A:OP1    | 1:AA:1006:C:N3      | 2.35                     | 0.60              |
| 1:AA:445:G:H2'     | 1:AA:446:G:H8       | 1.67                     | 0.60              |
| 1:AA:499:A:H4'     | 1:AA:500:G:OP1      | 2.02                     | 0.60              |
| 1:AA:664:G:H22     | 1:AA:741:G:H1       | 1.48                     | 0.60              |
| 2:AB:151:GLY:O     | 2:AB:153:ARG:N      | 2.35                     | 0.60              |
| 19:AS:41:VAL:C     | 19:AS:43:GLU:H      | 2.04                     | 0.60              |
| 24:AY:106:VAL:HG23 | 24:AY:132:ARG:HG3   | 1.84                     | 0.60              |
| 24:AY:293:THR:HB   | 24:AY:294:PRO:HD2   | 1.84                     | 0.60              |
| 26:B1:45:ASN:HD21  | 26:B1:47:GLN:NE2    | 1.98                     | 0.60              |
| 27:B2:47:ASN:ND2   | 35:BA:94(A):G:H21   | 2.00                     | 0.60              |
| 29:B4:27:THR:O     | 29:B4:28:LYS:HB3    | 2.02                     | 0.60              |
| 32:B7:34:ARG:HH12  | 32:B7:39:ARG:HD2    | 1.67                     | 0.60              |
| 33:B8:30:ARG:O     | 33:B8:31:HIS:HB3    | 2.01                     | 0.60              |
| 35:BA:1558:A:H4'   | 35:BA:1559:G:O5'    | 2.02                     | 0.60              |
| 35:BA:1833:U:H2'   | 35:BA:1834:U:H6     | 1.67                     | 0.60              |
| 35:BA:2348:U:H2'   | 35:BA:2349:G:H5''   | 1.83                     | 0.60              |
| 35:BA:389:G:O4'    | 35:BA:2413:G:H4'    | 2.02                     | 0.60              |
| 35:BA:2472:G:H3'   | 35:BA:2475:C:N4     | 2.17                     | 0.60              |
| 35:BA:975(A):G:O2' | 35:BA:976:C:H5'     | 2.02                     | 0.60              |
| 36:BB:106:G:H2'    | 36:BB:107:G:H8      | 1.65                     | 0.60              |
| 37:BC:14:LYS:H     | 37:BC:14:LYS:HD3    | 1.66                     | 0.60              |
| 42:BH:105:LEU:HD23 | 42:BH:105:LEU:H     | 1.67                     | 0.60              |
| 42:BH:170:ARG:O    | 42:BH:171:LEU:CB    | 2.47                     | 0.60              |
| 55:BW:59:VAL:O     | 55:BW:59:VAL:CG1    | 2.50                     | 0.60              |
| 56:BX:18:TYR:C     | 56:BX:20:GLY:H      | 2.05                     | 0.60              |
| 35:BA:484:C:OP1    | 57:BY:50:ARG:HG3    | 2.01                     | 0.60              |
| 1:CA:1004:A:H61    | 1:CA:1034:G:C2'     | 2.14                     | 0.60              |
| 1:CA:1108:G:H5'    | 3:CC:176:HIS:CD2    | 2.37                     | 0.60              |
| 1:CA:1441:G:H4'    | 1:CA:1442:G:C4      | 2.37                     | 0.60              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:201:C:H2'     | 1:CA:202:U:H5''   | 1.83                     | 0.60              |
| 1:CA:270:A:H2'     | 1:CA:271:C:C6     | 2.36                     | 0.60              |
| 4:CD:176:LEU:HD12  | 4:CD:177:ASP:H    | 1.66                     | 0.60              |
| 5:CE:6:PHE:HB3     | 5:CE:35:GLY:O     | 2.02                     | 0.60              |
| 17:CQ:48:GLU:O     | 17:CQ:49:GLU:C    | 2.39                     | 0.60              |
| 24:CY:71:THR:HG22  | 24:CY:80:ASN:OD1  | 2.01                     | 0.60              |
| 27:D2:69:ARG:CG    | 27:D2:70:GLN:H    | 2.15                     | 0.60              |
| 30:D5:36:CYS:SG    | 30:D5:38:ALA:HB3  | 2.42                     | 0.60              |
| 30:D5:3:LYS:NZ     | 35:DA:2613:U:H2'  | 2.16                     | 0.60              |
| 33:D8:25:MET:HG3   | 48:DP:64:LYS:CB   | 2.32                     | 0.60              |
| 34:D9:19:ARG:CB    | 35:DA:2756:U:H5'  | 2.31                     | 0.60              |
| 35:DA:134:C:H2'    | 35:DA:135:G:H8    | 1.65                     | 0.60              |
| 35:DA:1452:A:C3'   | 35:DA:1453:U:C5'  | 2.72                     | 0.60              |
| 35:DA:1899:G:H22   | 35:DA:1902:C:H41  | 1.21                     | 0.60              |
| 35:DA:2392:A:C8    | 48:DP:60:MET:HB3  | 2.34                     | 0.60              |
| 35:DA:2583:G:H2'   | 35:DA:2584:U:O2   | 2.02                     | 0.60              |
| 35:DA:2839:G:H1    | 35:DA:2878:U:H3   | 1.49                     | 0.60              |
| 35:DA:406:G:O2'    | 35:DA:407:G:H8    | 1.84                     | 0.60              |
| 35:DA:990:A:N6     | 35:DA:1186:G:H1'  | 2.17                     | 0.60              |
| 42:DH:170:ARG:O    | 42:DH:171:LEU:CB  | 2.49                     | 0.60              |
| 35:DA:910:A:H62    | 49:DQ:12:GLN:HA   | 1.67                     | 0.60              |
| 50:DR:10:LEU:HD22  | 50:DR:17:ARG:CD   | 2.32                     | 0.60              |
| 54:DV:47:VAL:HB    | 54:DV:50:PRO:O    | 2.01                     | 0.60              |
| 55:DW:68:ARG:CA    | 55:DW:110:LYS:HG2 | 2.32                     | 0.60              |
| 56:DX:10:ALA:O     | 56:DX:28:PHE:HB2  | 2.02                     | 0.60              |
| 57:DY:28:LYS:C     | 57:DY:38:ILE:HG22 | 2.20                     | 0.60              |
| 58:DZ:127:LYS:O    | 58:DZ:162:GLU:HG2 | 2.02                     | 0.60              |
| 1:AA:1148:U:H2'    | 1:AA:1149:C:O4'   | 2.02                     | 0.59              |
| 1:AA:1415:G:H2'    | 1:AA:1416:G:C8    | 2.37                     | 0.59              |
| 1:AA:853:G:O2'     | 1:AA:854:G:H5'    | 2.02                     | 0.59              |
| 2:AB:164:VAL:HG12  | 2:AB:165:VAL:N    | 2.16                     | 0.59              |
| 3:AC:25:GLY:C      | 3:AC:27:LYS:H     | 2.05                     | 0.59              |
| 5:AE:33:VAL:HG12   | 5:AE:34:VAL:N     | 2.16                     | 0.59              |
| 10:AJ:32:ALA:HB3   | 10:AJ:78:ASN:HD21 | 1.67                     | 0.59              |
| 12:AL:28:LYS:O     | 12:AL:29:GLY:C    | 2.38                     | 0.59              |
| 15:AO:76:GLU:C     | 15:AO:78:TYR:H    | 2.05                     | 0.59              |
| 18:AR:44:LEU:O     | 18:AR:45:SER:C    | 2.39                     | 0.59              |
| 24:AY:115:GLU:CD   | 24:AY:118:SER:HB3 | 2.22                     | 0.59              |
| 24:AY:201:ILE:H    | 24:AY:201:ILE:CD1 | 2.14                     | 0.59              |
| 24:AY:228:MET:O    | 24:AY:231:TYR:HB3 | 2.02                     | 0.59              |
| 24:AY:264:LEU:HD23 | 24:AY:264:LEU:O   | 2.01                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:B5:3:LYS:HG2    | 35:BA:747:U:O4     | 2.01                     | 0.59              |
| 35:BA:814:C:H2'    | 35:BA:815:C:H6     | 1.65                     | 0.59              |
| 40:BF:17:ARG:HG3   | 40:BF:17:ARG:HH11  | 1.67                     | 0.59              |
| 41:BG:114:ILE:HG12 | 41:BG:140:ILE:HG21 | 1.85                     | 0.59              |
| 46:BN:35:ARG:O     | 46:BN:36:GLY:C     | 2.39                     | 0.59              |
| 48:BP:23:PRO:HB2   | 48:BP:33:ARG:NE    | 2.16                     | 0.59              |
| 51:BS:99:LYS:O     | 51:BS:101:LEU:N    | 2.34                     | 0.59              |
| 52:BT:83:ILE:HG13  | 52:BT:84:GLN:HG2   | 1.83                     | 0.59              |
| 1:CA:1316:G:O2'    | 14:CN:18:VAL:HG11  | 2.02                     | 0.59              |
| 1:CA:483:C:C3'     | 1:CA:484:G:H5''    | 2.31                     | 0.59              |
| 4:CD:29:PRO:C      | 4:CD:30:LYS:HG2    | 2.21                     | 0.59              |
| 9:CI:126:SER:O     | 9:CI:128:ARG:HD2   | 2.02                     | 0.59              |
| 9:CI:3:GLN:NE2     | 9:CI:20:ARG:HH21   | 2.00                     | 0.59              |
| 9:CI:47:LEU:N      | 9:CI:47:LEU:CD1    | 2.64                     | 0.59              |
| 10:CJ:32:ALA:HB3   | 10:CJ:76:ASN:O     | 2.02                     | 0.59              |
| 10:CJ:3:LYS:NZ     | 10:CJ:77:PRO:HD2   | 2.17                     | 0.59              |
| 12:CL:47:LYS:HD2   | 12:CL:48:PRO:HD3   | 1.84                     | 0.59              |
| 20:CT:73:HIS:O     | 20:CT:76:ALA:HB3   | 2.02                     | 0.59              |
| 22:CW:31:G:H2'     | 22:CW:32:G:C8      | 2.34                     | 0.59              |
| 35:DA:1290:C:H2'   | 35:DA:1291:C:H6    | 1.67                     | 0.59              |
| 35:DA:1326:U:O2'   | 35:DA:1327:C:H5'   | 2.01                     | 0.59              |
| 35:DA:528:A:H2     | 35:DA:2043:C:C4'   | 2.15                     | 0.59              |
| 35:DA:2329:G:H2'   | 35:DA:2330:G:H8    | 1.67                     | 0.59              |
| 35:DA:2344:U:H4'   | 35:DA:2345:G:OP1   | 2.00                     | 0.59              |
| 35:DA:514:A:H2'    | 35:DA:515:A:C8     | 2.37                     | 0.59              |
| 35:DA:654(P):C:C2' | 35:DA:654(Q):C:H5' | 2.32                     | 0.59              |
| 38:DD:35:LYS:O     | 38:DD:36:PRO:C     | 2.40                     | 0.59              |
| 38:DD:43:ARG:HD2   | 38:DD:44:ASN:OD1   | 2.02                     | 0.59              |
| 35:DA:2052:G:H4'   | 39:DE:143:ASN:O    | 2.01                     | 0.59              |
| 42:DH:83:TYR:HB3   | 42:DH:135:GLY:N    | 2.17                     | 0.59              |
| 45:DL:19:UNK:C     | 45:DL:21:UNK:N     | 2.61                     | 0.59              |
| 51:DS:106:ARG:HB3  | 51:DS:106:ARG:NH1  | 2.13                     | 0.59              |
| 52:DT:51:ARG:HG3   | 52:DT:98:LYS:HE3   | 1.83                     | 0.59              |
| 47:DO:64:ARG:NE    | 52:DT:70:VAL:HG21  | 2.17                     | 0.59              |
| 57:DY:74:PRO:HG3   | 57:DY:83:THR:HG22  | 1.84                     | 0.59              |
| 58:DZ:179:ASP:OD1  | 58:DZ:182:LYS:HG3  | 2.02                     | 0.59              |
| 1:AA:999:C:H2'     | 1:AA:1000:U:C6     | 2.37                     | 0.59              |
| 1:AA:1208:C:H2'    | 1:AA:1209:C:C6     | 2.37                     | 0.59              |
| 1:AA:390:C:H2'     | 1:AA:391:G:H8      | 1.66                     | 0.59              |
| 3:AC:94:LEU:O      | 3:AC:95:THR:HG23   | 2.01                     | 0.59              |
| 6:AF:69:GLU:H      | 6:AF:69:GLU:CD     | 2.06                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:AJ:32:ALA:N     | 10:AJ:78:ASN:ND2   | 2.49                     | 0.59              |
| 13:AM:27:LYS:HE2   | 13:AM:31:LYS:CE    | 2.24                     | 0.59              |
| 14:AN:14:PRO:O     | 14:AN:15:LYS:O     | 2.19                     | 0.59              |
| 16:AP:20:VAL:HG21  | 16:AP:32:TYR:CG    | 2.36                     | 0.59              |
| 22:AW:10:G:H2'     | 22:AW:11:A:C8      | 2.37                     | 0.59              |
| 24:AY:337:SER:CA   | 24:AY:355:LEU:HD23 | 2.32                     | 0.59              |
| 27:B2:67:LYS:O     | 27:B2:70:GLN:HG3   | 2.02                     | 0.59              |
| 31:B6:35:GLU:HB2   | 31:B6:51:GLU:HB2   | 1.84                     | 0.59              |
| 32:B7:24:THR:HG23  | 32:B7:27:GLY:N     | 2.16                     | 0.59              |
| 35:BA:1361:G:O2'   | 35:BA:1362:C:H5'   | 2.03                     | 0.59              |
| 35:BA:1438:U:O2'   | 35:BA:1439:A:H5'   | 2.01                     | 0.59              |
| 35:BA:2498:C:O2'   | 35:BA:2499:C:H5'   | 2.03                     | 0.59              |
| 37:BC:4:HIS:ND1    | 37:BC:8:TYR:CE2    | 2.70                     | 0.59              |
| 39:BE:34:VAL:HG11  | 39:BE:78:LEU:HD22  | 1.84                     | 0.59              |
| 40:BF:140:LEU:O    | 40:BF:143:ALA:HB3  | 2.03                     | 0.59              |
| 40:BF:195:ASP:CG   | 40:BF:196:LEU:H    | 2.06                     | 0.59              |
| 42:BH:105:LEU:HD23 | 42:BH:113:VAL:HB   | 1.84                     | 0.59              |
| 46:BN:67:LEU:CD2   | 46:BN:87:LEU:HB3   | 2.32                     | 0.59              |
| 48:BP:16:ARG:HD3   | 48:BP:16:ARG:C     | 2.22                     | 0.59              |
| 50:BR:97:VAL:HA    | 50:BR:113:LEU:O    | 2.00                     | 0.59              |
| 36:BB:7:G:H5'      | 51:BS:29:PHE:CD1   | 2.36                     | 0.59              |
| 57:BY:31:LEU:HB2   | 57:BY:32:PRO:CA    | 2.31                     | 0.59              |
| 1:CA:1270:C:H4'    | 1:CA:1313:U:O2'    | 2.02                     | 0.59              |
| 1:CA:183:G:H2'     | 1:CA:184:G:H8      | 1.65                     | 0.59              |
| 2:CB:24:TRP:CZ3    | 2:CB:26:PRO:HA     | 2.38                     | 0.59              |
| 6:CF:1:MET:HE1     | 6:CF:68:PRO:HD3    | 1.84                     | 0.59              |
| 9:CI:53:VAL:C      | 9:CI:55:ALA:H      | 2.05                     | 0.59              |
| 13:CM:11:ARG:O     | 13:CM:13:LYS:N     | 2.35                     | 0.59              |
| 24:CY:164:MET:HB2  | 24:CY:258:VAL:O    | 2.01                     | 0.59              |
| 24:CY:499:ARG:HB2  | 24:CY:506:GLN:HB3  | 1.84                     | 0.59              |
| 24:CY:74:TRP:HB3   | 24:CY:79:ILE:HD11  | 1.83                     | 0.59              |
| 35:DA:1022:G:N2    | 35:DA:1142(A):A:H2 | 2.00                     | 0.59              |
| 35:DA:1842:G:H2'   | 35:DA:1843:C:C6    | 2.37                     | 0.59              |
| 35:DA:2037:G:H2'   | 35:DA:2038:G:C8    | 2.38                     | 0.59              |
| 35:DA:2260:C:H2'   | 35:DA:2261:C:H6    | 1.67                     | 0.59              |
| 35:DA:2756:U:H1'   | 35:DA:2757:A:C8    | 2.37                     | 0.59              |
| 36:DB:40:U:O2      | 36:DB:43:C:H5''    | 2.02                     | 0.59              |
| 41:DG:77:ILE:O     | 41:DG:80:PHE:N     | 2.32                     | 0.59              |
| 44:DK:3:LYS:HD3    | 44:DK:29:GLN:HG2   | 1.84                     | 0.59              |
| 45:DL:100:UNK:HA   | 45:DL:105:UNK:CB   | 2.31                     | 0.59              |
| 48:DP:16:ARG:C     | 48:DP:16:ARG:HD3   | 2.23                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 49:DQ:52:VAL:O    | 49:DQ:55:VAL:HG12  | 2.02                     | 0.59              |
| 56:DX:8:ILE:HD11  | 56:DX:42:ALA:O     | 2.02                     | 0.59              |
| 58:DZ:20:ARG:NH1  | 58:DZ:20:ARG:HB2   | 2.13                     | 0.59              |
| 1:AA:1095:U:P     | 1:AA:1108:G:H1     | 2.25                     | 0.59              |
| 1:AA:992:U:H1'    | 1:AA:993:G:C2      | 2.37                     | 0.59              |
| 2:AB:233:SER:CB   | 2:AB:234:PRO:CD    | 2.80                     | 0.59              |
| 4:AD:15:GLU:O     | 4:AD:17:VAL:HG23   | 2.01                     | 0.59              |
| 8:AH:12:ARG:NH1   | 8:AH:27:PRO:HD3    | 2.18                     | 0.59              |
| 9:AI:79:LEU:CD1   | 9:AI:83:ARG:HB2    | 2.33                     | 0.59              |
| 10:AJ:29:ARG:CZ   | 10:AJ:29:ARG:HB3   | 2.31                     | 0.59              |
| 12:AL:28:LYS:HE2  | 12:AL:33:ARG:NH1   | 2.17                     | 0.59              |
| 17:AQ:52:LYS:CD   | 17:AQ:52:LYS:H     | 2.12                     | 0.59              |
| 22:AW:74:A:H2'    | 22:AW:75:C:H5''    | 1.83                     | 0.59              |
| 24:AY:135:PHE:CD1 | 24:AY:272:LEU:HD22 | 2.37                     | 0.59              |
| 24:AY:97:SER:O    | 24:AY:100:VAL:HG13 | 2.02                     | 0.59              |
| 33:B8:48:PHE:C    | 33:B8:49:VAL:HG22  | 2.21                     | 0.59              |
| 34:B9:17:ILE:HG22 | 34:B9:18:ARG:N     | 2.17                     | 0.59              |
| 34:B9:19:ARG:CB   | 35:BA:2756:U:H5'   | 2.32                     | 0.59              |
| 35:BA:1328:G:O5'  | 35:BA:1328:G:H8    | 1.85                     | 0.59              |
| 35:BA:1921:G:O2'  | 35:BA:1922:G:H5'   | 2.02                     | 0.59              |
| 35:BA:212:G:C5'   | 35:BA:212:G:H8     | 2.16                     | 0.59              |
| 42:BH:65:HIS:HE1  | 42:BH:69:ARG:HH11  | 1.50                     | 0.59              |
| 35:BA:1141:U:H6   | 46:BN:63:THR:HG21  | 1.67                     | 0.59              |
| 52:BT:11:GLU:C    | 52:BT:13:ARG:H     | 2.06                     | 0.59              |
| 57:BY:61:ILE:HG12 | 57:BY:62:GLU:N     | 2.16                     | 0.59              |
| 1:CA:950:U:H2'    | 1:CA:951:G:H8      | 1.67                     | 0.59              |
| 8:CH:86:ILE:HG12  | 8:CH:135:CYS:HA    | 1.84                     | 0.59              |
| 10:CJ:30:SER:HA   | 10:CJ:80:LYS:HE2   | 1.85                     | 0.59              |
| 22:CW:37:U:H3     | 23:CX:13:A:N6      | 2.00                     | 0.59              |
| 23:CX:13:A:H5'    | 23:CX:14:A:OP2     | 2.03                     | 0.59              |
| 24:CY:537:GLU:O   | 24:CY:540:PRO:HD2  | 2.02                     | 0.59              |
| 24:CY:578:SER:HB3 | 24:CY:581:ALA:CB   | 2.31                     | 0.59              |
| 30:D5:3:LYS:HZ2   | 30:D5:5:PRO:HB2    | 1.67                     | 0.59              |
| 31:D6:5:VAL:HG12  | 31:D6:6:ARG:N      | 2.16                     | 0.59              |
| 35:DA:1362:C:O2'  | 35:DA:1363:C:H5'   | 2.01                     | 0.59              |
| 35:DA:1788:C:O2'  | 35:DA:1789:A:H5'   | 2.03                     | 0.59              |
| 35:DA:2462:U:H2'  | 35:DA:2463:C:C6    | 2.37                     | 0.59              |
| 35:DA:2469:A:H2   | 35:DA:2481:G:H21   | 1.49                     | 0.59              |
| 35:DA:2646:C:OP2  | 35:DA:2732:G:H2'   | 2.01                     | 0.59              |
| 39:DE:24:THR:HG22 | 39:DE:186:GLY:CA   | 2.30                     | 0.59              |
| 41:DG:51:ARG:NE   | 41:DG:51:ARG:HA    | 2.13                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 42:DH:98:LEU:HD22  | 42:DH:125:VAL:HG23  | 1.83                     | 0.59              |
| 46:DN:67:LEU:HB3   | 46:DN:88:GLU:HG3    | 1.83                     | 0.59              |
| 48:DP:16:ARG:HD3   | 48:DP:18:ARG:N      | 2.09                     | 0.59              |
| 49:DQ:27:VAL:HG11  | 49:DQ:134:ARG:HD3   | 1.83                     | 0.59              |
| 51:DS:59:LYS:HG2   | 51:DS:60:GLY:N      | 2.17                     | 0.59              |
| 52:DT:28:VAL:CG1   | 52:DT:46:GLU:HA     | 2.31                     | 0.59              |
| 57:DY:105:ALA:C    | 57:DY:107:ASP:H     | 2.02                     | 0.59              |
| 57:DY:27:VAL:HG12  | 57:DY:29:GLU:OE1    | 2.02                     | 0.59              |
| 2:AB:21:ARG:HD2    | 2:AB:39:ILE:CG1     | 2.33                     | 0.59              |
| 8:AH:104:ARG:HB3   | 8:AH:108:GLY:H      | 1.67                     | 0.59              |
| 12:AL:76:ASN:CG    | 12:AL:76:ASN:O      | 2.41                     | 0.59              |
| 13:AM:74:VAL:HA    | 13:AM:77:ASN:HD22   | 1.67                     | 0.59              |
| 21:AU:6:ARG:HH21   | 21:AU:15:ARG:NH2    | 1.99                     | 0.59              |
| 24:AY:82:ILE:HD12  | 24:AY:101:LEU:HD22  | 1.85                     | 0.59              |
| 29:B4:9:LEU:CD1    | 29:B4:10:VAL:H      | 2.15                     | 0.59              |
| 31:B6:40:CYS:HB2   | 31:B6:46:HIS:ND1    | 2.18                     | 0.59              |
| 31:B6:7:ILE:N      | 31:B6:7:ILE:HD12    | 2.17                     | 0.59              |
| 33:B8:61:LEU:C     | 33:B8:63:PRO:HD2    | 2.22                     | 0.59              |
| 35:BA:139(A):G:N2  | 56:BX:44:GLU:OE1    | 2.36                     | 0.59              |
| 35:BA:2040:C:H2'   | 35:BA:2041:U:H6     | 1.67                     | 0.59              |
| 31:B6:54:ILE:HD13  | 35:BA:2420:C:H4'    | 1.83                     | 0.59              |
| 35:BA:2469:A:H2    | 35:BA:2481:G:H21    | 1.49                     | 0.59              |
| 35:BA:2801:A:H4'   | 35:BA:2801(A):A:O4' | 2.02                     | 0.59              |
| 35:BA:786:C:O2'    | 35:BA:787:U:H5'     | 2.02                     | 0.59              |
| 38:BD:35:LYS:CD    | 38:BD:36:PRO:N      | 2.60                     | 0.59              |
| 39:BE:45:THR:O     | 39:BE:46:ALA:HB2    | 2.02                     | 0.59              |
| 39:BE:49:LEU:CD2   | 39:BE:49:LEU:N      | 2.66                     | 0.59              |
| 41:BG:59:GLU:O     | 41:BG:63:ILE:HG13   | 2.03                     | 0.59              |
| 48:BP:23:PRO:O     | 48:BP:33:ARG:HD2    | 2.01                     | 0.59              |
| 48:BP:33:ARG:O     | 48:BP:34:GLY:C      | 2.40                     | 0.59              |
| 48:BP:58:THR:C     | 48:BP:61:ARG:HE     | 2.06                     | 0.59              |
| 49:BQ:43:THR:O     | 49:BQ:47:ILE:HG13   | 2.02                     | 0.59              |
| 51:BS:89:ARG:HG3   | 51:BS:92:TYR:CB     | 2.31                     | 0.59              |
| 58:BZ:165:VAL:HG12 | 58:BZ:166:SER:N     | 2.17                     | 0.59              |
| 1:CA:1005:A:OP1    | 1:CA:1006:C:N3      | 2.35                     | 0.59              |
| 1:CA:953:G:O6      | 1:CA:1228:C:N4      | 2.35                     | 0.59              |
| 1:CA:218:C:H5'     | 1:CA:470:C:N4       | 2.18                     | 0.59              |
| 3:CC:86:VAL:O      | 3:CC:90:GLU:HG2     | 2.02                     | 0.59              |
| 4:CD:58:LEU:C      | 4:CD:58:LEU:HD23    | 2.22                     | 0.59              |
| 5:CE:11:ILE:HD12   | 5:CE:31:LEU:CD1     | 2.32                     | 0.59              |
| 13:CM:63:THR:HG22  | 13:CM:64:TRP:H      | 1.67                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 13:CM:83:ASP:CG     | 13:CM:84:ILE:H      | 2.06                     | 0.59              |
| 15:CO:55:GLY:HA2    | 15:CO:58:MET:HE3    | 1.84                     | 0.59              |
| 22:CW:14:A:C3'      | 22:CW:15:G:H5''     | 2.33                     | 0.59              |
| 22:CW:74:A:C3'      | 22:CW:75:C:H5''     | 2.32                     | 0.59              |
| 24:CY:406:GLU:HB3   | 24:CY:407:PRO:HD2   | 1.84                     | 0.59              |
| 24:CY:499:ARG:O     | 24:CY:505:GLY:O     | 2.19                     | 0.59              |
| 25:D0:73:GLY:C      | 25:D0:75:LEU:H      | 2.06                     | 0.59              |
| 26:D1:6:GLU:C       | 26:D1:7:ILE:HD12    | 2.22                     | 0.59              |
| 35:DA:16:G:H2'      | 35:DA:17:G:H8       | 1.67                     | 0.59              |
| 35:DA:2287:A:N6     | 35:DA:2344:U:N3     | 2.48                     | 0.59              |
| 35:DA:2787:C:H1'    | 39:DE:61:ARG:CG     | 2.30                     | 0.59              |
| 36:DB:18:G:H2'      | 36:DB:19:G:H8       | 1.67                     | 0.59              |
| 37:DC:99:GLU:O      | 37:DC:100:ILE:HD13  | 2.03                     | 0.59              |
| 38:DD:267:SER:O     | 38:DD:269:PHE:N     | 2.34                     | 0.59              |
| 39:DE:170:LEU:HD12  | 39:DE:170:LEU:N     | 2.17                     | 0.59              |
| 41:DG:114:ILE:O     | 41:DG:116:ASP:N     | 2.36                     | 0.59              |
| 42:DH:105:LEU:CD2   | 42:DH:113:VAL:HB    | 2.32                     | 0.59              |
| 47:DO:104:ARG:NE    | 52:DT:33:LYS:HE3    | 2.16                     | 0.59              |
| 56:DX:18:TYR:C      | 56:DX:20:GLY:H      | 2.05                     | 0.59              |
| 57:DY:17:SER:OG     | 57:DY:18:GLY:N      | 2.35                     | 0.59              |
| 57:DY:76:CYS:SG     | 57:DY:77:PRO:CD     | 2.82                     | 0.59              |
| 4:AD:121:VAL:HA     | 4:AD:126:ILE:HD13   | 1.83                     | 0.59              |
| 4:AD:108:LEU:HD21   | 4:AD:183:GLY:HA3    | 1.84                     | 0.59              |
| 5:AE:107:ARG:HG2    | 5:AE:108:ALA:N      | 2.18                     | 0.59              |
| 7:AG:113:GLU:HG2    | 7:AG:119:ARG:HG2    | 1.85                     | 0.59              |
| 9:AI:41:VAL:O       | 9:AI:41:VAL:HG12    | 2.02                     | 0.59              |
| 19:AS:6:LYS:HG2     | 19:AS:7:LYS:CE      | 2.32                     | 0.59              |
| 22:AV:3:C:C2'       | 22:AV:4:G:H5'       | 2.32                     | 0.59              |
| 24:AY:206:LEU:HD11  | 24:AY:210:ARG:HH12  | 1.67                     | 0.59              |
| 24:AY:315:LYS:NZ    | 24:AY:317:MET:HG2   | 2.17                     | 0.59              |
| 31:B6:16:CYS:SG     | 31:B6:48:VAL:HG21   | 2.42                     | 0.59              |
| 35:BA:1102:C:H2'    | 35:BA:1103:A:C8     | 2.37                     | 0.59              |
| 35:BA:1221(A):C:O2' | 35:BA:1222:C:H5'    | 2.02                     | 0.59              |
| 35:BA:2712:U:H1'    | 35:BA:2712(A):A:C8  | 2.37                     | 0.59              |
| 35:BA:2712:U:O2'    | 35:BA:2712(A):A:O5' | 2.20                     | 0.59              |
| 35:BA:654(R):C:HO2' | 35:BA:654(S):G:H8   | 1.49                     | 0.59              |
| 35:BA:892:G:H2'     | 35:BA:893:C:C6      | 2.37                     | 0.59              |
| 38:BD:145:VAL:HG12  | 38:BD:146:GLU:N     | 2.14                     | 0.59              |
| 38:BD:106:ILE:HD11  | 38:BD:196:VAL:HG13  | 1.83                     | 0.59              |
| 40:BF:163:VAL:O     | 40:BF:166:ALA:HB3   | 2.03                     | 0.59              |
| 40:BF:18:ARG:HG2    | 40:BF:19:GLU:H      | 1.68                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:BK:3:LYS:HB3    | 44:BK:29:GLN:HB3   | 1.84                     | 0.59              |
| 51:BS:88:ASP:CG    | 51:BS:89:ARG:N     | 2.55                     | 0.59              |
| 52:BT:11:GLU:H     | 52:BT:11:GLU:CD    | 2.06                     | 0.59              |
| 55:BW:68:ARG:CA    | 55:BW:110:LYS:HG2  | 2.32                     | 0.59              |
| 57:BY:9:LYS:HD3    | 57:BY:94:LYS:HE2   | 1.84                     | 0.59              |
| 58:BZ:151:HIS:CA   | 58:BZ:171:ILE:HG23 | 2.22                     | 0.59              |
| 36:BB:106:G:C5'    | 58:BZ:31:ARG:HB3   | 2.33                     | 0.59              |
| 1:CA:99:U:H2'      | 1:CA:100:C:C6      | 2.37                     | 0.59              |
| 10:CJ:18:ALA:C     | 10:CJ:20:ALA:H     | 2.06                     | 0.59              |
| 10:CJ:47:PHE:CZ    | 14:CN:37:PHE:CE2   | 2.90                     | 0.59              |
| 11:CK:18:ARG:HH21  | 11:CK:37:GLY:N     | 2.00                     | 0.59              |
| 12:CL:47:LYS:HZ2   | 12:CL:47:LYS:HB3   | 1.67                     | 0.59              |
| 24:CY:555:LEU:HD21 | 24:CY:599:PRO:HG3  | 1.84                     | 0.59              |
| 27:D2:65:ASN:ND2   | 35:DA:112:U:H5'    | 2.17                     | 0.59              |
| 29:D4:25:TYR:O     | 29:D4:26:SER:HB3   | 2.03                     | 0.59              |
| 35:DA:1102:C:H2'   | 35:DA:1103:A:C8    | 2.38                     | 0.59              |
| 35:DA:1198:U:O2    | 35:DA:1198:U:H2'   | 2.01                     | 0.59              |
| 35:DA:15:G:O2'     | 35:DA:16:G:H5'     | 2.02                     | 0.59              |
| 35:DA:2008:C:H2'   | 35:DA:2009:G:H8    | 1.67                     | 0.59              |
| 35:DA:214:G:H1'    | 35:DA:216:A:O2'    | 2.02                     | 0.59              |
| 35:DA:274:G:O2'    | 35:DA:275:G:H5''   | 2.03                     | 0.59              |
| 35:DA:303:U:H2'    | 35:DA:304:G:C8     | 2.38                     | 0.59              |
| 35:DA:637:A:OP1    | 48:DP:133:SER:HB3  | 2.03                     | 0.59              |
| 40:DF:32:LEU:O     | 40:DF:36:VAL:HG23  | 2.01                     | 0.59              |
| 42:DH:41:MET:HG2   | 42:DH:43:VAL:HG13  | 1.84                     | 0.59              |
| 35:DA:1080:C:O2'   | 44:DK:126:MET:HG3  | 2.02                     | 0.59              |
| 46:DN:21:LYS:HD2   | 46:DN:26:LEU:HB3   | 1.85                     | 0.59              |
| 48:DP:91:PHE:HZ    | 48:DP:100:LEU:HD11 | 1.67                     | 0.59              |
| 52:DT:125:ARG:HH11 | 52:DT:125:ARG:CA   | 2.14                     | 0.59              |
| 54:DV:18:LEU:CG    | 54:DV:19:LYS:H     | 2.14                     | 0.59              |
| 58:DZ:61:LEU:HD12  | 58:DZ:65:GLN:HB2   | 1.85                     | 0.59              |
| 58:DZ:61:LEU:C     | 58:DZ:63:ASP:H     | 2.06                     | 0.59              |
| 1:AA:1347:G:O2'    | 1:AA:1348:U:P      | 2.60                     | 0.59              |
| 1:AA:1409:C:H2'    | 1:AA:1410:G:H8     | 1.68                     | 0.59              |
| 2:AB:172:ILE:H     | 2:AB:172:ILE:CD1   | 2.04                     | 0.59              |
| 5:AE:42:GLY:HA3    | 5:AE:66:MET:HG2    | 1.83                     | 0.59              |
| 12:AL:20:LYS:N     | 12:AL:20:LYS:HD3   | 2.16                     | 0.59              |
| 13:AM:106:ASN:O    | 13:AM:107:ALA:HB3  | 2.02                     | 0.59              |
| 22:AV:72:A:H2'     | 22:AV:73:A:C8      | 2.37                     | 0.59              |
| 22:AW:30:G:H2'     | 22:AW:31:G:H8      | 1.65                     | 0.59              |
| 26:B1:32:LYS:C     | 26:B1:33:LYS:HG3   | 2.21                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 35:BA:2756:U:H1'    | 35:BA:2757:A:C8    | 2.37                     | 0.59              |
| 35:BA:310:A:OP2     | 57:BY:18:GLY:HA2   | 2.02                     | 0.59              |
| 35:BA:27:G:N2       | 35:BA:512:G:C2'    | 2.64                     | 0.59              |
| 35:BA:614(A):U:H5'' | 35:BA:614(B):G:OP1 | 2.03                     | 0.59              |
| 35:BA:752:A:O2'     | 35:BA:753:C:OP2    | 2.18                     | 0.59              |
| 35:BA:996:A:O3'     | 53:BU:92:ARG:HG2   | 2.03                     | 0.59              |
| 29:B4:3:GLU:HG3     | 36:BB:43:C:OP1     | 2.03                     | 0.59              |
| 38:BD:11:PRO:O      | 38:BD:13:ARG:N     | 2.36                     | 0.59              |
| 40:BF:133:ASN:H     | 40:BF:162:LEU:HD23 | 1.66                     | 0.59              |
| 40:BF:84:VAL:O      | 40:BF:86:GLY:N     | 2.34                     | 0.59              |
| 47:BO:4:PRO:O       | 47:BO:5:GLN:CB     | 2.51                     | 0.59              |
| 51:BS:97:ARG:C      | 51:BS:97:ARG:NE    | 2.56                     | 0.59              |
| 58:BZ:145:GLU:O     | 58:BZ:146:ILE:C    | 2.39                     | 0.59              |
| 1:CA:1381:U:C5      | 1:CA:1382:C:C5     | 2.90                     | 0.59              |
| 1:CA:1444:C:H2'     | 1:CA:1445:C:C5     | 2.37                     | 0.59              |
| 2:CB:96:ARG:N       | 2:CB:96:ARG:HD2    | 2.18                     | 0.59              |
| 10:CJ:94:VAL:HG12   | 10:CJ:95:GLU:N     | 2.17                     | 0.59              |
| 12:CL:20:LYS:N      | 12:CL:20:LYS:HD3   | 2.17                     | 0.59              |
| 12:CL:24:VAL:HG13   | 12:CL:98:TYR:CE2   | 2.37                     | 0.59              |
| 17:CQ:52:LYS:H      | 17:CQ:52:LYS:CD    | 2.11                     | 0.59              |
| 22:CW:14:A:H2'      | 22:CW:15:G:H5''    | 1.85                     | 0.59              |
| 1:CA:358:U:H4'      | 24:CY:322:VAL:O    | 2.02                     | 0.59              |
| 24:CY:388:THR:HG23  | 24:CY:399:LEU:HD22 | 1.83                     | 0.59              |
| 30:D5:56:LYS:HG3    | 30:D5:57:VAL:N     | 2.11                     | 0.59              |
| 35:DA:1467:C:C5     | 35:DA:1546:C:H2'   | 2.38                     | 0.59              |
| 35:DA:1428:C:N4     | 35:DA:1569:A:H3'   | 2.18                     | 0.59              |
| 35:DA:212:G:H8      | 35:DA:212:G:C5'    | 2.15                     | 0.59              |
| 35:DA:2443:C:H2'    | 35:DA:2443:C:O2    | 2.02                     | 0.59              |
| 35:DA:2473:U:C3'    | 35:DA:2474:C:H5''  | 2.14                     | 0.59              |
| 35:DA:975(A):G:O2'  | 35:DA:976:C:H5'    | 2.01                     | 0.59              |
| 38:DD:201:HIS:O     | 38:DD:204:ILE:HG12 | 2.03                     | 0.59              |
| 46:DN:133:GLN:HG2   | 46:DN:134:ARG:N    | 2.17                     | 0.59              |
| 48:DP:114:ILE:O     | 48:DP:130:PHE:HA   | 2.02                     | 0.59              |
| 49:DQ:97:VAL:HG11   | 49:DQ:103:MET:HE1  | 1.84                     | 0.59              |
| 30:D5:55:ARG:HH12   | 50:DR:33:ARG:HD2   | 1.67                     | 0.59              |
| 54:DV:35:LEU:O      | 54:DV:37:VAL:N     | 2.36                     | 0.59              |
| 1:AA:1190:G:H3'     | 3:AC:3:ASN:HD22    | 1.67                     | 0.59              |
| 3:AC:70:VAL:CG1     | 3:AC:72:LYS:H      | 2.06                     | 0.59              |
| 3:AC:79:ARG:CB      | 3:AC:79:ARG:HH11   | 2.11                     | 0.59              |
| 8:AH:86:ILE:HG12    | 8:AH:135:CYS:HA    | 1.83                     | 0.59              |
| 17:AQ:53:LEU:HD21   | 17:AQ:85:VAL:HG11  | 1.84                     | 0.59              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 18:AR:74:ARG:HD3   | 18:AR:81:PHE:CD2    | 2.37                     | 0.59              |
| 24:AY:529:ILE:HD11 | 24:AY:567:LEU:HD11  | 1.84                     | 0.59              |
| 24:AY:662:LYS:HZ2  | 42:BH:175:LYS:CE    | 2.10                     | 0.59              |
| 29:B4:2:LYS:O      | 29:B4:4:GLY:N       | 2.33                     | 0.59              |
| 35:BA:1203:G:H3'   | 35:BA:1204:A:C5'    | 2.31                     | 0.59              |
| 35:BA:2188:C:H2'   | 35:BA:2189:U:C6     | 2.38                     | 0.59              |
| 35:BA:688:U:H4'    | 35:BA:1780:A:C2     | 2.37                     | 0.59              |
| 38:BD:134:ARG:HG3  | 38:BD:135:PHE:CD1   | 2.37                     | 0.59              |
| 42:BH:12:PRO:CD    | 42:BH:49:VAL:HG12   | 2.24                     | 0.59              |
| 52:BT:90:GLN:HG2   | 52:BT:120:ARG:NH2   | 2.17                     | 0.59              |
| 6:CF:37:VAL:O      | 6:CF:38:GLU:HG3     | 2.03                     | 0.59              |
| 7:CG:64:GLN:O      | 7:CG:67:GLU:HB3     | 2.02                     | 0.59              |
| 1:CA:1226:C:N4     | 13:CM:104:ARG:HD2   | 2.17                     | 0.59              |
| 24:CY:213:HIS:O    | 24:CY:217:VAL:HG23  | 2.03                     | 0.59              |
| 24:CY:71:THR:HG21  | 24:CY:357:ARG:HD2   | 1.83                     | 0.59              |
| 24:CY:530:VAL:O    | 24:CY:531:GLY:C     | 2.41                     | 0.59              |
| 29:D4:5:ILE:HG12   | 29:D4:5:ILE:O       | 2.01                     | 0.59              |
| 31:D6:45:LYS:HE3   | 35:DA:2371:G:H5''   | 1.85                     | 0.59              |
| 31:D6:51:GLU:HG2   | 31:D6:52:VAL:H      | 1.68                     | 0.59              |
| 35:DA:1049:C:H2'   | 35:DA:1050:A:H8     | 1.67                     | 0.59              |
| 35:DA:1163:G:O2'   | 35:DA:1164:G:H5'    | 2.03                     | 0.59              |
| 35:DA:1212:G:O2'   | 35:DA:1236:G:N2     | 2.35                     | 0.59              |
| 35:DA:1993:U:H4'   | 39:DE:128:SER:OG    | 2.02                     | 0.59              |
| 35:DA:2801:A:H4'   | 35:DA:2801(A):A:O4' | 2.02                     | 0.59              |
| 39:DE:36:ARG:HG2   | 39:DE:36:ARG:NH1    | 2.14                     | 0.59              |
| 40:DF:158:THR:HG21 | 40:DF:163:VAL:HB    | 1.85                     | 0.59              |
| 40:DF:17:ARG:HH11  | 40:DF:17:ARG:HG3    | 1.68                     | 0.59              |
| 40:DF:110:LEU:CD1  | 40:DF:206:ILE:HD11  | 2.25                     | 0.59              |
| 41:DG:40:ASN:ND2   | 41:DG:41:GLN:N      | 2.51                     | 0.59              |
| 47:DO:4:PRO:O      | 47:DO:5:GLN:CB      | 2.51                     | 0.59              |
| 49:DQ:12:GLN:NE2   | 49:DQ:73:PRO:HD2    | 2.16                     | 0.59              |
| 35:DA:2495:G:H5''  | 49:DQ:82:ARG:HG2    | 1.84                     | 0.59              |
| 52:DT:29:ARG:CG    | 52:DT:85:LYS:HA     | 2.33                     | 0.59              |
| 57:DY:90:LEU:HD12  | 57:DY:91:GLU:OE2    | 2.03                     | 0.59              |
| 58:DZ:142:SER:H    | 58:DZ:144:LEU:CD2   | 2.16                     | 0.59              |
| 2:AB:7:VAL:O       | 2:AB:11:LEU:HG      | 2.02                     | 0.59              |
| 17:AQ:80:GLY:O     | 17:AQ:81:ARG:HD2    | 2.02                     | 0.59              |
| 24:AY:196:ILE:HG13 | 24:AY:197:ARG:N     | 2.17                     | 0.59              |
| 35:BA:1168:G:H2'   | 35:BA:1169:G:C8     | 2.37                     | 0.59              |
| 35:BA:1405:U:H2'   | 35:BA:1406:U:C6     | 2.38                     | 0.59              |
| 35:BA:2111:C:C2    | 35:BA:2147:G:N2     | 2.71                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 35:BA:2233:U:H2'   | 35:BA:2234:G:C8     | 2.37                     | 0.59              |
| 35:BA:2506:U:H4'   | 35:BA:2507:C:OP1    | 2.00                     | 0.59              |
| 35:BA:274:G:O2'    | 35:BA:275:G:H5''    | 2.01                     | 0.59              |
| 35:BA:2794:C:H42   | 35:BA:2801(A):A:H61 | 1.50                     | 0.59              |
| 35:BA:675:A:OP1    | 40:BF:63:LYS:HE2    | 2.03                     | 0.59              |
| 41:BG:130:ASN:OD1  | 41:BG:160:VAL:HA    | 2.02                     | 0.59              |
| 41:BG:131:TYR:CE2  | 41:BG:133:LEU:HB3   | 2.38                     | 0.59              |
| 41:BG:91:ARG:C     | 41:BG:91:ARG:HD2    | 2.23                     | 0.59              |
| 42:BH:171:LEU:CD2  | 42:BH:171:LEU:C     | 2.71                     | 0.59              |
| 47:BO:61:VAL:HG21  | 47:BO:111:PHE:CE2   | 2.38                     | 0.59              |
| 48:BP:80:TYR:CE1   | 48:BP:111:ARG:HG2   | 2.38                     | 0.59              |
| 35:BA:1242:A:C6    | 48:BP:8:PRO:HG2     | 2.38                     | 0.59              |
| 49:BQ:21:THR:HG23  | 49:BQ:101:ARG:HB2   | 1.85                     | 0.59              |
| 52:BT:90:GLN:O     | 52:BT:91:ARG:C      | 2.40                     | 0.59              |
| 58:BZ:107:THR:HG23 | 58:BZ:111:VAL:HG21  | 1.83                     | 0.59              |
| 58:BZ:152:ALA:HA   | 58:BZ:167:PRO:HB2   | 1.84                     | 0.59              |
| 1:CA:122:G:O2'     | 1:CA:123:C:H5'      | 2.03                     | 0.59              |
| 1:CA:630:G:O2'     | 1:CA:631:G:H5''     | 2.03                     | 0.59              |
| 2:CB:111:ARG:HG2   | 2:CB:111:ARG:HH11   | 1.67                     | 0.59              |
| 1:CA:1190:G:H3'    | 3:CC:3:ASN:HD22     | 1.68                     | 0.59              |
| 5:CE:42:GLY:HA3    | 5:CE:66:MET:HG2     | 1.83                     | 0.59              |
| 7:CG:121:ALA:O     | 7:CG:125:MET:HG3    | 2.03                     | 0.59              |
| 10:CJ:29:ARG:HB3   | 10:CJ:29:ARG:CZ     | 2.32                     | 0.59              |
| 16:CP:25:ARG:HG3   | 16:CP:25:ARG:NH1    | 2.18                     | 0.59              |
| 35:DA:1093:G:H21   | 35:DA:1098:A:H62    | 1.50                     | 0.59              |
| 35:DA:1361:G:O2'   | 35:DA:1362:C:H5'    | 2.02                     | 0.59              |
| 35:DA:1711:C:O2'   | 35:DA:1712:C:H5'    | 2.03                     | 0.59              |
| 37:DC:29:LEU:HD23  | 37:DC:29:LEU:C      | 2.22                     | 0.59              |
| 39:DE:184:VAL:O    | 39:DE:186:GLY:N     | 2.28                     | 0.59              |
| 40:DF:39:TRP:CB    | 40:DF:101:LEU:HD22  | 2.32                     | 0.59              |
| 42:DH:12:PRO:CD    | 42:DH:49:VAL:HG12   | 2.24                     | 0.59              |
| 46:DN:128:HIS:HE1  | 46:DN:134:ARG:HH11  | 1.50                     | 0.59              |
| 51:DS:98:VAL:HG12  | 51:DS:100:ALA:HB2   | 1.85                     | 0.59              |
| 57:DY:43:ASN:ND2   | 57:DY:64:GLU:HG3    | 2.17                     | 0.59              |
| 1:AA:1347:G:O2'    | 1:AA:1348:U:OP2     | 2.21                     | 0.59              |
| 3:AC:58:GLU:H      | 3:AC:65:ALA:CB      | 2.09                     | 0.59              |
| 6:AF:42:GLU:O      | 6:AF:44:GLY:N       | 2.36                     | 0.59              |
| 6:AF:1:MET:HE1     | 6:AF:68:PRO:HD3     | 1.85                     | 0.59              |
| 12:AL:27:LEU:HG    | 12:AL:62:SER:HB2    | 1.85                     | 0.59              |
| 16:AP:21:VAL:HG11  | 16:AP:59:TRP:NE1    | 2.18                     | 0.59              |
| 16:AP:50:LYS:O     | 16:AP:51:VAL:HG23   | 2.03                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:AR:37:VAL:O     | 18:AR:39:VAL:N     | 2.36                     | 0.59              |
| 20:AT:84:LEU:C     | 20:AT:86:ARG:H     | 2.06                     | 0.59              |
| 24:AY:413:ILE:HG22 | 24:AY:449:THR:O    | 2.02                     | 0.59              |
| 24:AY:487:ILE:HD13 | 24:AY:487:ILE:H    | 1.68                     | 0.59              |
| 24:AY:606:MET:O    | 24:AY:646:PHE:HA   | 2.02                     | 0.59              |
| 35:BA:1169:G:H1    | 35:BA:1180:C:H42   | 1.49                     | 0.59              |
| 35:BA:1930:G:O2'   | 35:BA:1931:U:P     | 2.61                     | 0.59              |
| 35:BA:2495:G:H5''  | 49:BQ:82:ARG:HG2   | 1.85                     | 0.59              |
| 35:BA:2891:G:H4'   | 35:BA:2892:A:OP1   | 2.01                     | 0.59              |
| 35:BA:363(A):A:H2' | 35:BA:363(B):G:H8  | 1.68                     | 0.59              |
| 38:BD:24:ILE:O     | 38:BD:25:THR:O     | 2.20                     | 0.59              |
| 40:BF:32:LEU:O     | 40:BF:36:VAL:HG23  | 2.03                     | 0.59              |
| 41:BG:85:GLY:C     | 41:BG:87:PRO:HD3   | 2.22                     | 0.59              |
| 45:BM:5:UNK:C      | 45:BM:7:UNK:N      | 3.27                     | 0.59              |
| 46:BN:41:ASP:C     | 53:BU:64:ARG:HH22  | 2.05                     | 0.59              |
| 49:BQ:24:GLY:O     | 49:BQ:102:VAL:HG23 | 2.02                     | 0.59              |
| 52:BT:129:ARG:CG   | 52:BT:129:ARG:O    | 2.50                     | 0.59              |
| 1:CA:1054:C:OP2    | 1:CA:1197:G:OP2    | 2.20                     | 0.59              |
| 1:CA:1490:C:C5'    | 1:CA:1490:C:H6     | 2.13                     | 0.59              |
| 1:CA:275:G:H5''    | 17:CQ:14:LYS:CB    | 2.32                     | 0.59              |
| 1:CA:277:C:O2'     | 1:CA:278:G:H5'     | 2.02                     | 0.59              |
| 1:CA:313:A:O2'     | 1:CA:314:C:H5'     | 2.03                     | 0.59              |
| 1:CA:434:U:H2'     | 1:CA:435:C:C6      | 2.38                     | 0.59              |
| 1:CA:72:C:H2'      | 1:CA:73:G:C8       | 2.37                     | 0.59              |
| 2:CB:164:VAL:HG12  | 2:CB:165:VAL:N     | 2.17                     | 0.59              |
| 2:CB:193:ASP:O     | 2:CB:193:ASP:OD2   | 2.20                     | 0.59              |
| 2:CB:204:ASN:HD22  | 2:CB:206:ASP:H     | 1.49                     | 0.59              |
| 3:CC:99:VAL:HG23   | 3:CC:99:VAL:O      | 2.03                     | 0.59              |
| 6:CF:36:ARG:CZ     | 6:CF:36:ARG:HB3    | 2.31                     | 0.59              |
| 9:CI:4:TYR:HA      | 9:CI:88:TYR:CE1    | 2.38                     | 0.59              |
| 15:CO:65:ARG:HH11  | 15:CO:65:ARG:HG2   | 1.67                     | 0.59              |
| 19:CS:21:GLU:HG3   | 19:CS:22:LEU:HD23  | 1.84                     | 0.59              |
| 24:CY:223:PHE:CE2  | 24:CY:249:GLY:HA3  | 2.38                     | 0.59              |
| 24:CY:388:THR:C    | 24:CY:389:LEU:HD12 | 2.22                     | 0.59              |
| 29:D4:2:LYS:O      | 29:D4:4:GLY:N      | 2.35                     | 0.59              |
| 33:D8:6:THR:HG22   | 33:D8:63:PRO:HD3   | 1.83                     | 0.59              |
| 35:DA:1847:A:H3'   | 35:DA:1848:A:H5'   | 1.84                     | 0.59              |
| 35:DA:1858:G:H2'   | 35:DA:1883:G:H22   | 1.66                     | 0.59              |
| 35:DA:451:C:H41    | 35:DA:453:C:H3'    | 1.68                     | 0.59              |
| 35:DA:519:U:H5''   | 55:DW:25:ARG:NH2   | 2.17                     | 0.59              |
| 35:DA:650:C:H2'    | 35:DA:651:G:H5''   | 1.85                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:DC:26:ALA:O     | 37:DC:30:VAL:HG23  | 2.03                     | 0.59              |
| 29:D4:24:THR:HG21  | 41:DG:104:GLU:HG2  | 1.84                     | 0.59              |
| 55:DW:17:VAL:O     | 55:DW:20:VAL:HG22  | 2.03                     | 0.59              |
| 1:AA:1279:A:H5'    | 1:AA:1280:A:OP1    | 2.03                     | 0.59              |
| 1:AA:1521:G:H2'    | 1:AA:1522:U:C6     | 2.38                     | 0.59              |
| 1:AA:183:G:H2'     | 1:AA:184:G:H8      | 1.67                     | 0.59              |
| 4:AD:129:ASN:HD21  | 4:AD:145:GLU:N     | 1.96                     | 0.59              |
| 6:AF:38:GLU:O      | 6:AF:39:LYS:O      | 2.20                     | 0.59              |
| 24:AY:414:GLU:O    | 24:AY:474:ALA:HB1  | 2.03                     | 0.59              |
| 30:B5:43:HIS:HD2   | 35:BA:2815:C:O2'   | 1.85                     | 0.59              |
| 31:B6:18:ARG:HG3   | 31:B6:19:ARG:H     | 1.68                     | 0.59              |
| 35:BA:1711:C:O2'   | 35:BA:1712:C:H5'   | 2.03                     | 0.59              |
| 35:BA:2745:C:H2'   | 35:BA:2746:U:C6    | 2.38                     | 0.59              |
| 35:BA:528:A:H2     | 35:BA:2043:C:C5'   | 2.15                     | 0.59              |
| 36:BB:20:C:H2'     | 36:BB:21:G:H5'     | 1.84                     | 0.59              |
| 38:BD:9:TYR:C      | 38:BD:10:THR:HG22  | 2.23                     | 0.59              |
| 38:BD:241:PRO:O    | 38:BD:242:ARG:HB2  | 2.02                     | 0.59              |
| 39:BE:52:LEU:O     | 39:BE:74:PRO:HA    | 2.03                     | 0.59              |
| 40:BF:148:LEU:HD23 | 40:BF:191:ARG:NH1  | 2.18                     | 0.59              |
| 40:BF:185:ASP:OD1  | 40:BF:188:ARG:HD3  | 2.03                     | 0.59              |
| 48:BP:91:PHE:N     | 48:BP:91:PHE:CD1   | 2.67                     | 0.59              |
| 48:BP:97:PRO:HD3   | 48:BP:126:VAL:O    | 2.03                     | 0.59              |
| 49:BQ:27:VAL:HG11  | 49:BQ:134:ARG:HD3  | 1.84                     | 0.59              |
| 52:BT:57:PHE:C     | 52:BT:58:ASN:HD22  | 2.06                     | 0.59              |
| 35:BA:2018:G:H21   | 53:BU:34:LYS:NZ    | 2.00                     | 0.59              |
| 54:BV:18:LEU:CG    | 54:BV:19:LYS:H     | 2.15                     | 0.59              |
| 57:BY:2:ARG:N      | 57:BY:4:LYS:HG2    | 2.18                     | 0.59              |
| 58:BZ:108:PRO:HB3  | 58:BZ:141:VAL:CG1  | 2.33                     | 0.59              |
| 58:BZ:99:TYR:CE2   | 58:BZ:125:LEU:HD13 | 2.37                     | 0.59              |
| 1:CA:960:U:C5      | 1:CA:1225:A:C8     | 2.91                     | 0.59              |
| 1:CA:1463:C:O2'    | 1:CA:1464:G:H5'    | 2.02                     | 0.59              |
| 1:CA:882:C:O2'     | 1:CA:883:C:H5'     | 2.03                     | 0.59              |
| 9:CI:93:ARG:C      | 9:CI:95:LYS:H      | 2.06                     | 0.59              |
| 10:CJ:55:LYS:H     | 10:CJ:55:LYS:HE3   | 1.68                     | 0.59              |
| 19:CS:21:GLU:HG3   | 19:CS:22:LEU:CD2   | 2.33                     | 0.59              |
| 24:CY:109:ASP:OD1  | 24:CY:111:SER:HB2  | 2.02                     | 0.59              |
| 24:CY:142:THR:HG22 | 24:CY:143:GLY:N    | 2.17                     | 0.59              |
| 24:CY:85:PRO:O     | 24:CY:87:HIS:N     | 2.36                     | 0.59              |
| 25:D0:14:ARG:CB    | 25:D0:14:ARG:HH11  | 2.15                     | 0.59              |
| 35:DA:1109:C:H5'   | 35:DA:1110:G:OP2   | 2.03                     | 0.59              |
| 35:DA:2030:A:H5''  | 35:DA:2031:A:OP1   | 2.02                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:2097:C:H2'   | 35:DA:2098:U:H6    | 1.67                     | 0.59              |
| 35:DA:296:C:O2'    | 35:DA:297:C:H5'    | 2.03                     | 0.59              |
| 35:DA:443:A:H3'    | 40:DF:45:ARG:HH21  | 1.67                     | 0.59              |
| 35:DA:492:A:C2'    | 35:DA:493:G:H5'    | 2.33                     | 0.59              |
| 35:DA:564:C:O2'    | 35:DA:565:C:H5'    | 2.03                     | 0.59              |
| 37:DC:57:GLN:NE2   | 37:DC:205:ALA:HA   | 2.18                     | 0.59              |
| 38:DD:267:SER:HA   | 38:DD:270:ILE:HD11 | 1.84                     | 0.59              |
| 40:DF:125:LEU:HD23 | 40:DF:125:LEU:N    | 2.17                     | 0.59              |
| 40:DF:59:TYR:HE1   | 40:DF:85:GLY:O     | 1.85                     | 0.59              |
| 41:DG:91:ARG:HD2   | 41:DG:92:VAL:N     | 2.18                     | 0.59              |
| 42:DH:92:ILE:O     | 42:DH:94:TYR:N     | 2.30                     | 0.59              |
| 44:DK:37:PHE:O     | 44:DK:41:PHE:HB3   | 2.02                     | 0.59              |
| 45:DL:67:UNK:O     | 45:DL:69:UNK:N     | 2.36                     | 0.59              |
| 47:DO:47:ILE:CG2   | 47:DO:48:PRO:HD2   | 2.33                     | 0.59              |
| 47:DO:91:LEU:N     | 47:DO:91:LEU:HD22  | 2.18                     | 0.59              |
| 50:DR:28:LEU:CD2   | 50:DR:29:LEU:HD12  | 2.32                     | 0.59              |
| 55:DW:9:TYR:H      | 55:DW:102:HIS:HD2  | 1.50                     | 0.59              |
| 35:DA:143:G:H4'    | 56:DX:35:THR:HG21  | 1.83                     | 0.59              |
| 1:AA:1410:G:H2'    | 1:AA:1411:C:H6     | 1.68                     | 0.58              |
| 1:AA:313:A:O2'     | 1:AA:314:C:H5'     | 2.03                     | 0.58              |
| 1:AA:405:U:H3'     | 1:AA:406:G:H5'     | 1.84                     | 0.58              |
| 1:AA:861:G:O2'     | 1:AA:862:C:H5'     | 2.02                     | 0.58              |
| 10:AJ:94:VAL:HG12  | 10:AJ:95:GLU:N     | 2.17                     | 0.58              |
| 24:AY:510:VAL:HG13 | 24:AY:569:ASP:O    | 2.02                     | 0.58              |
| 24:AY:544:LYS:O    | 24:AY:548:GLU:HB2  | 2.03                     | 0.58              |
| 24:AY:519:ARG:NH1  | 24:AY:678:GLU:HB2  | 2.18                     | 0.58              |
| 25:B0:10:THR:HG22  | 25:B0:11:ARG:H     | 1.68                     | 0.58              |
| 25:B0:14:ARG:CB    | 25:B0:14:ARG:HH11  | 2.15                     | 0.58              |
| 26:B1:57:GLU:HG2   | 26:B1:58:ILE:N     | 2.18                     | 0.58              |
| 26:B1:41:ARG:HH22  | 35:BA:1365:A:C5'   | 2.16                     | 0.58              |
| 35:BA:279:C:H3'    | 35:BA:280:C:H5''   | 1.84                     | 0.58              |
| 35:BA:605:C:H2'    | 35:BA:606:U:H6     | 1.67                     | 0.58              |
| 38:BD:130:ALA:C    | 38:BD:131:LEU:HD12 | 2.24                     | 0.58              |
| 38:BD:31:LYS:NZ    | 38:BD:33:LEU:HB2   | 2.18                     | 0.58              |
| 39:BE:9:VAL:CG2    | 39:BE:10:GLY:N     | 2.65                     | 0.58              |
| 42:BH:83:TYR:HB3   | 42:BH:135:GLY:N    | 2.16                     | 0.58              |
| 42:BH:68:THR:O     | 42:BH:72:ILE:HG12  | 2.03                     | 0.58              |
| 49:BQ:39:PRO:HB3   | 49:BQ:99:PRO:HD3   | 1.85                     | 0.58              |
| 52:BT:28:VAL:HG21  | 52:BT:46:GLU:CG    | 2.26                     | 0.58              |
| 52:BT:35:LYS:NZ    | 52:BT:41:ARG:NH1   | 2.50                     | 0.58              |
| 57:BY:43:ASN:ND2   | 57:BY:64:GLU:HG3   | 2.17                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 58:BZ:4:ARG:HH12  | 58:BZ:66:SER:CB    | 2.15                     | 0.58              |
| 58:BZ:54:HIS:HE1  | 58:BZ:123:ASP:OD2  | 1.85                     | 0.58              |
| 1:CA:100:C:H2'    | 1:CA:101:A:C8      | 2.38                     | 0.58              |
| 1:CA:499:A:H4'    | 1:CA:500:G:OP1     | 2.02                     | 0.58              |
| 6:CF:36:ARG:NH1   | 6:CF:36:ARG:HB3    | 2.18                     | 0.58              |
| 6:CF:4:TYR:CE1    | 6:CF:92:LYS:HD2    | 2.38                     | 0.58              |
| 8:CH:5:PRO:O      | 8:CH:8:ASP:HB3     | 2.02                     | 0.58              |
| 1:CA:1308:U:H5''  | 13:CM:98:VAL:CG2   | 2.32                     | 0.58              |
| 20:CT:84:LEU:C    | 20:CT:86:ARG:H     | 2.06                     | 0.58              |
| 24:CY:181:LEU:CD2 | 24:CY:243:VAL:HG22 | 2.30                     | 0.58              |
| 24:CY:416:LYS:HG2 | 24:CY:417:THR:N    | 2.19                     | 0.58              |
| 24:CY:515:GLU:OE2 | 24:CY:564:LYS:HD3  | 2.03                     | 0.58              |
| 35:DA:1203:G:H3'  | 35:DA:1204:A:C5'   | 2.33                     | 0.58              |
| 35:DA:1525:G:H2'  | 35:DA:1526:G:C8    | 2.38                     | 0.58              |
| 35:DA:2262:U:C2'  | 35:DA:2263:C:H5''  | 2.31                     | 0.58              |
| 35:DA:358:U:H2'   | 35:DA:359:A:C8     | 2.27                     | 0.58              |
| 35:DA:1245:G:C5'  | 40:DF:34:TRP:HZ2   | 2.16                     | 0.58              |
| 51:DS:99:LYS:O    | 51:DS:101:LEU:N    | 2.36                     | 0.58              |
| 52:DT:51:ARG:O    | 52:DT:61:PHE:HA    | 2.03                     | 0.58              |
| 1:AA:1016:A:H2'   | 1:AA:1017:G:O4'    | 2.02                     | 0.58              |
| 1:AA:1348:U:H2'   | 1:AA:1349:A:H8     | 1.67                     | 0.58              |
| 1:AA:241:C:O2'    | 1:AA:242:C:H5'     | 2.03                     | 0.58              |
| 1:AA:434:U:H2'    | 1:AA:435:C:C6      | 2.38                     | 0.58              |
| 1:AA:741:G:O2'    | 1:AA:742:G:H5'     | 2.03                     | 0.58              |
| 1:AA:812:C:O2'    | 1:AA:813:U:OP2     | 2.20                     | 0.58              |
| 4:AD:102:ASP:HB3  | 4:AD:136:PRO:HB3   | 1.84                     | 0.58              |
| 5:AE:100:VAL:HG23 | 5:AE:100:VAL:O     | 2.02                     | 0.58              |
| 5:AE:11:ILE:HD12  | 5:AE:31:LEU:CD1    | 2.32                     | 0.58              |
| 1:AA:1298:C:H5''  | 7:AG:114:ARG:HH22  | 1.69                     | 0.58              |
| 9:AI:4:TYR:HA     | 9:AI:88:TYR:CE1    | 2.38                     | 0.58              |
| 9:AI:93:ARG:C     | 9:AI:95:LYS:H      | 2.06                     | 0.58              |
| 14:AN:44:LEU:HD12 | 14:AN:44:LEU:O     | 2.03                     | 0.58              |
| 15:AO:64:ARG:HG3  | 15:AO:64:ARG:HH11  | 1.69                     | 0.58              |
| 24:AY:137:ASN:ND2 | 24:AY:263:ALA:H    | 2.00                     | 0.58              |
| 35:BA:1290:C:H2'  | 35:BA:1291:C:C6    | 2.38                     | 0.58              |
| 35:BA:1467:C:C5   | 35:BA:1546:C:H2'   | 2.38                     | 0.58              |
| 35:BA:1485:G:N3   | 35:BA:1505:C:N3    | 2.51                     | 0.58              |
| 35:BA:1796:U:OP1  | 38:BD:276:LYS:HE3  | 2.03                     | 0.58              |
| 35:BA:184:C:H2'   | 35:BA:185:U:H6     | 1.65                     | 0.58              |
| 35:BA:320:A:H4'   | 35:BA:322:A:C8     | 2.38                     | 0.58              |
| 35:BA:365:C:C6    | 35:BA:365:C:H5'    | 2.37                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:519:U:H5''   | 55:BW:25:ARG:NH2   | 2.18                     | 0.58              |
| 35:BA:6:A:N3       | 35:BA:6:A:H2'      | 2.17                     | 0.58              |
| 27:B2:3:LEU:HB2    | 35:BA:98:G:OP1     | 2.02                     | 0.58              |
| 36:BB:18:G:H2'     | 36:BB:19:G:H8      | 1.68                     | 0.58              |
| 42:BH:86:GLU:HA    | 42:BH:132:ARG:HA   | 1.84                     | 0.58              |
| 46:BN:97:ARG:O     | 46:BN:101:HIS:HB2  | 2.03                     | 0.58              |
| 55:BW:109:GLU:CD   | 55:BW:109:GLU:H    | 2.07                     | 0.58              |
| 58:BZ:109:ALA:C    | 58:BZ:111:VAL:N    | 2.57                     | 0.58              |
| 1:CA:1305:G:N2     | 1:CA:1331:G:O2'    | 2.30                     | 0.58              |
| 1:CA:1370:G:C2     | 1:CA:1371:G:C8     | 2.91                     | 0.58              |
| 1:CA:1429:C:H2'    | 1:CA:1430:C:C6     | 2.38                     | 0.58              |
| 1:CA:853:G:O2'     | 1:CA:854:G:H5'     | 2.03                     | 0.58              |
| 1:CA:1298:C:H5''   | 7:CG:114:ARG:HH22  | 1.68                     | 0.58              |
| 12:CL:27:LEU:HG    | 12:CL:62:SER:HB2   | 1.85                     | 0.58              |
| 16:CP:20:VAL:HG21  | 16:CP:32:TYR:CG    | 2.37                     | 0.58              |
| 19:CS:29:ARG:O     | 19:CS:31:ILE:N     | 2.35                     | 0.58              |
| 24:CY:110:SER:HA   | 24:CY:149:VAL:CG2  | 2.33                     | 0.58              |
| 24:CY:137:ASN:O    | 24:CY:139:MET:N    | 2.30                     | 0.58              |
| 24:CY:183:MET:O    | 24:CY:201:ILE:HD11 | 2.03                     | 0.58              |
| 24:CY:227:ILE:HD13 | 24:CY:242:LEU:HA   | 1.85                     | 0.58              |
| 24:CY:485:GLU:OE2  | 24:CY:553:GLY:HA3  | 2.02                     | 0.58              |
| 25:D0:10:THR:HG22  | 25:D0:11:ARG:H     | 1.68                     | 0.58              |
| 35:DA:1353:A:H2'   | 35:DA:1354:A:C8    | 2.38                     | 0.58              |
| 35:DA:1493:C:C4    | 35:DA:2206:G:O2'   | 2.56                     | 0.58              |
| 35:DA:1614:A:H2'   | 35:DA:1615:C:H5'   | 1.84                     | 0.58              |
| 35:DA:1717:G:C2'   | 35:DA:1718:G:H5''  | 2.34                     | 0.58              |
| 35:DA:1794:U:O2'   | 35:DA:1795:C:H5'   | 2.03                     | 0.58              |
| 30:D5:19:ARG:HA    | 35:DA:2046:G:C5'   | 2.32                     | 0.58              |
| 35:DA:2056:G:H2'   | 35:DA:2056:G:N3    | 2.17                     | 0.58              |
| 35:DA:2200:C:H42   | 35:DA:2223:G:H1    | 1.51                     | 0.58              |
| 35:DA:2233:U:H2'   | 35:DA:2234:G:C8    | 2.39                     | 0.58              |
| 35:DA:271(I):G:H3' | 35:DA:271(J):C:H6  | 1.68                     | 0.58              |
| 35:DA:27:G:O2'     | 35:DA:28:A:H8      | 1.85                     | 0.58              |
| 37:DC:211:ARG:HG3  | 37:DC:211:ARG:HH11 | 1.68                     | 0.58              |
| 38:DD:80:ALA:HB3   | 38:DD:94:LEU:HB3   | 1.85                     | 0.58              |
| 39:DE:101:ARG:HH11 | 39:DE:169:ASN:ND2  | 2.01                     | 0.58              |
| 42:DH:16:SER:CB    | 42:DH:27:LYS:HB2   | 2.31                     | 0.58              |
| 54:DV:32:THR:OG1   | 54:DV:60:GLU:HG3   | 2.04                     | 0.58              |
| 1:AA:160:A:H1'     | 1:AA:344:A:N7      | 2.18                     | 0.58              |
| 1:AA:483:C:C3'     | 1:AA:484:G:H5''    | 2.29                     | 0.58              |
| 1:AA:955:U:O2'     | 1:AA:956:U:H5'     | 2.03                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:AD:203:VAL:O     | 4:AD:206:PHE:HB3   | 2.03                     | 0.58              |
| 4:AD:25:ARG:HH12   | 4:AD:30:LYS:HB2    | 1.69                     | 0.58              |
| 4:AD:61:LYS:HD3    | 4:AD:206:PHE:CE2   | 2.38                     | 0.58              |
| 24:AY:101:LEU:HD12 | 24:AY:103:GLY:O    | 2.04                     | 0.58              |
| 24:AY:71:THR:HG21  | 24:AY:357:ARG:HD2  | 1.83                     | 0.58              |
| 19:AS:64:GLU:C     | 29:B4:48:ARG:HH22  | 2.07                     | 0.58              |
| 29:B4:9:LEU:HD13   | 29:B4:26:SER:O     | 2.02                     | 0.58              |
| 35:BA:1332:G:H22   | 35:BA:1609:A:H3'   | 1.68                     | 0.58              |
| 42:BH:98:LEU:HD22  | 42:BH:125:VAL:HG23 | 1.83                     | 0.58              |
| 35:BA:637:A:OP1    | 48:BP:133:SER:HB3  | 2.03                     | 0.58              |
| 33:B8:25:MET:HG3   | 48:BP:64:LYS:CB    | 2.33                     | 0.58              |
| 56:BX:8:ILE:HD11   | 56:BX:42:ALA:O     | 2.02                     | 0.58              |
| 58:BZ:145:GLU:OE1  | 58:BZ:146:ILE:HD13 | 2.03                     | 0.58              |
| 1:CA:1452:C:O2'    | 1:CA:1456:G:H5''   | 2.03                     | 0.58              |
| 1:CA:160:A:H1'     | 1:CA:344:A:N7      | 2.18                     | 0.58              |
| 1:CA:59:A:H2'      | 1:CA:59:A:N3       | 2.17                     | 0.58              |
| 2:CB:97:TRP:CZ2    | 2:CB:102:LEU:HD13  | 2.34                     | 0.58              |
| 2:CB:151:GLY:O     | 2:CB:153:ARG:N     | 2.36                     | 0.58              |
| 20:CT:47:GLY:O     | 20:CT:49:ALA:N     | 2.30                     | 0.58              |
| 24:CY:498:ILE:HG13 | 24:CY:498:ILE:O    | 2.03                     | 0.58              |
| 24:CY:605:ILE:HD11 | 24:CY:677:GLN:CG   | 2.32                     | 0.58              |
| 26:D1:3:LYS:HD3    | 35:DA:1364:G:H5''  | 1.84                     | 0.58              |
| 26:D1:80:LEU:HB3   | 26:D1:82:LEU:CD1   | 2.33                     | 0.58              |
| 26:D1:82:LEU:HD23  | 26:D1:90:ILE:HG23  | 1.85                     | 0.58              |
| 27:D2:36:ARG:HA    | 27:D2:39:ALA:CB    | 2.33                     | 0.58              |
| 35:DA:1196:C:O2'   | 35:DA:1227:G:H4'   | 2.04                     | 0.58              |
| 35:DA:145:G:H2'    | 35:DA:146:G:C8     | 2.37                     | 0.58              |
| 35:DA:1485:G:N3    | 35:DA:1505:C:N3    | 2.50                     | 0.58              |
| 35:DA:1827:C:C2'   | 35:DA:1828:G:H5'   | 2.32                     | 0.58              |
| 35:DA:528:A:H2     | 35:DA:2043:C:C5'   | 2.15                     | 0.58              |
| 35:DA:2297:C:O2'   | 35:DA:2298:A:H5'   | 2.03                     | 0.58              |
| 35:DA:484:C:OP1    | 57:DY:50:ARG:HG3   | 2.03                     | 0.58              |
| 35:DA:27:G:N2      | 35:DA:512:G:C2'    | 2.64                     | 0.58              |
| 35:DA:573:G:O2'    | 35:DA:574:C:H3'    | 2.03                     | 0.58              |
| 35:DA:813:U:H2'    | 35:DA:814:C:C5     | 2.38                     | 0.58              |
| 35:DA:889:C:H2'    | 35:DA:890:A:O4'    | 2.03                     | 0.58              |
| 36:DB:48:A:H2'     | 36:DB:49:C:C6      | 2.37                     | 0.58              |
| 40:DF:24:LEU:HB3   | 40:DF:25:PRO:CD    | 2.32                     | 0.58              |
| 35:DA:797:C:OP1    | 40:DF:62:ARG:HG3   | 2.02                     | 0.58              |
| 41:DG:133:LEU:HD12 | 41:DG:133:LEU:O    | 2.02                     | 0.58              |
| 42:DH:156:ALA:O    | 42:DH:158:HIS:HD2  | 1.86                     | 0.58              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 48:DP:80:TYR:CE1    | 48:DP:111:ARG:HG2  | 2.37                     | 0.58              |
| 52:DT:108:ARG:HA    | 52:DT:111:ARG:NH1  | 2.18                     | 0.58              |
| 53:DU:49:HIS:HA     | 53:DU:52:ARG:HB2   | 1.84                     | 0.58              |
| 53:DU:93:LYS:HD2    | 53:DU:93:LYS:H     | 1.69                     | 0.58              |
| 57:DY:9:LYS:HD3     | 57:DY:94:LYS:HE2   | 1.83                     | 0.58              |
| 58:DZ:58:VAL:HA     | 58:DZ:67:LEU:O     | 2.03                     | 0.58              |
| 1:AA:1392:G:N2      | 1:AA:1502:A:C8     | 2.71                     | 0.58              |
| 1:AA:218:C:H5'      | 1:AA:470:C:N4      | 2.18                     | 0.58              |
| 1:AA:219:C:H2'      | 1:AA:220:G:O4'     | 2.02                     | 0.58              |
| 17:AQ:48:GLU:O      | 17:AQ:50:LYS:N     | 2.35                     | 0.58              |
| 19:AS:46:GLY:N      | 19:AS:62:ILE:HG23  | 2.18                     | 0.58              |
| 22:AW:68:C:H2'      | 22:AW:69:C:C5      | 2.38                     | 0.58              |
| 24:AY:108:PHE:HE1   | 24:AY:118:SER:HB2  | 1.67                     | 0.58              |
| 24:AY:227:ILE:HD13  | 24:AY:242:LEU:HA   | 1.85                     | 0.58              |
| 30:B5:43:HIS:CD2    | 35:BA:2815:C:O2'   | 2.56                     | 0.58              |
| 35:BA:2809:A:H2'    | 35:BA:2810:A:C8    | 2.39                     | 0.58              |
| 35:BA:552:G:H8      | 35:BA:552:G:H5'    | 1.68                     | 0.58              |
| 35:BA:654(P):C:C2'  | 35:BA:654(Q):C:H5' | 2.32                     | 0.58              |
| 36:BB:115:G:H2'     | 36:BB:116:G:H8     | 1.69                     | 0.58              |
| 38:BD:34:VAL:C      | 38:BD:36:PRO:HD2   | 2.24                     | 0.58              |
| 41:BG:107:LEU:HD23  | 41:BG:111:LEU:CD1  | 2.32                     | 0.58              |
| 42:BH:12:PRO:O      | 42:BH:15:VAL:HG22  | 2.04                     | 0.58              |
| 52:BT:108:ARG:HA    | 52:BT:111:ARG:NH1  | 2.18                     | 0.58              |
| 52:BT:28:VAL:CG1    | 52:BT:46:GLU:HA    | 2.33                     | 0.58              |
| 52:BT:85:LYS:HZ3    | 52:BT:85:LYS:HB3   | 1.64                     | 0.58              |
| 1:CA:38:G:C2        | 1:CA:397:A:C2      | 2.92                     | 0.58              |
| 1:CA:8:A:N6         | 4:CD:209:ARG:HB2   | 2.17                     | 0.58              |
| 6:CF:11:ASN:HB3     | 6:CF:14:LEU:HG     | 1.83                     | 0.58              |
| 7:CG:140:ASP:O      | 7:CG:144:MET:HG2   | 2.04                     | 0.58              |
| 10:CJ:78:ASN:HB2    | 10:CJ:81:THR:HG23  | 1.85                     | 0.58              |
| 13:CM:49:THR:HB     | 13:CM:52:GLU:HG3   | 1.85                     | 0.58              |
| 18:CR:44:LEU:O      | 18:CR:45:SER:C     | 2.39                     | 0.58              |
| 30:D5:44:THR:O      | 30:D5:51:TYR:HE1   | 1.87                     | 0.58              |
| 31:D6:9:LEU:HD12    | 31:D6:28:ARG:HG3   | 1.84                     | 0.58              |
| 31:D6:11:LEU:CD2    | 31:D6:51:GLU:HG3   | 2.32                     | 0.58              |
| 35:DA:1221(A):C:O2' | 35:DA:1222:C:H5'   | 2.03                     | 0.58              |
| 35:DA:1308:A:H2'    | 35:DA:1309:G:O4'   | 2.02                     | 0.58              |
| 35:DA:1799:G:H8     | 38:DD:181:GLU:OE1  | 1.87                     | 0.58              |
| 35:DA:1949:G:H2'    | 35:DA:1950:G:C8    | 2.38                     | 0.58              |
| 35:DA:570:G:H2'     | 35:DA:2030:A:C5    | 2.38                     | 0.58              |
| 35:DA:2506:U:H4'    | 35:DA:2507:C:OP1   | 2.02                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:DA:2439:A:HO2' | 35:DA:2587:A:H5''  | 1.64                     | 0.58              |
| 35:DA:2662:A:H2'  | 35:DA:2663:G:O4'   | 2.03                     | 0.58              |
| 35:DA:2809:A:H2'  | 35:DA:2810:A:C8    | 2.38                     | 0.58              |
| 42:DH:171:LEU:CD2 | 42:DH:171:LEU:C    | 2.71                     | 0.58              |
| 43:DJ:37:UNK:C    | 43:DJ:39:UNK:N     | 2.65                     | 0.58              |
| 52:DT:27:THR:O    | 52:DT:28:VAL:CG2   | 2.48                     | 0.58              |
| 52:DT:90:GLN:O    | 52:DT:91:ARG:C     | 2.41                     | 0.58              |
| 53:DU:8:VAL:HG23  | 53:DU:11:ARG:HH21  | 1.68                     | 0.58              |
| 58:DZ:9:TYR:OH    | 58:DZ:61:LEU:HD13  | 2.04                     | 0.58              |
| 1:AA:99:U:H2'     | 1:AA:100:C:C6      | 2.38                     | 0.58              |
| 2:AB:12:GLU:HA    | 2:AB:16:HIS:ND1    | 2.17                     | 0.58              |
| 2:AB:21:ARG:HB3   | 2:AB:39:ILE:HA     | 1.86                     | 0.58              |
| 4:AD:29:PRO:C     | 4:AD:30:LYS:HG2    | 2.23                     | 0.58              |
| 24:AY:108:PHE:CE1 | 24:AY:118:SER:HB2  | 2.37                     | 0.58              |
| 26:B1:26:ARG:HG3  | 26:B1:27:GLU:N     | 2.17                     | 0.58              |
| 27:B2:3:LEU:HD22  | 27:B2:7:ARG:CZ     | 2.33                     | 0.58              |
| 33:B8:16:ILE:HD12 | 33:B8:57:ARG:HG2   | 1.85                     | 0.58              |
| 33:B8:61:LEU:CD1  | 33:B8:62:LEU:H     | 2.10                     | 0.58              |
| 35:BA:16:G:O2'    | 35:BA:17:G:H5'     | 2.03                     | 0.58              |
| 35:BA:1815:A:OP2  | 35:BA:1822:G:H5''  | 2.03                     | 0.58              |
| 35:BA:192:C:C2'   | 35:BA:193:U:H5'    | 2.29                     | 0.58              |
| 35:BA:570:G:H2'   | 35:BA:2030:A:C5    | 2.39                     | 0.58              |
| 35:BA:2454:G:C2'  | 35:BA:2455:G:H5'   | 2.32                     | 0.58              |
| 35:BA:2646:C:OP2  | 35:BA:2732:G:H2'   | 2.02                     | 0.58              |
| 35:BA:2742:C:C2'  | 35:BA:2743:C:H5'   | 2.33                     | 0.58              |
| 35:BA:274:G:H2'   | 35:BA:274:G:N3     | 2.18                     | 0.58              |
| 35:BA:285:C:H2'   | 35:BA:286:C:H5'    | 1.86                     | 0.58              |
| 35:BA:303:U:H2'   | 35:BA:304:G:C8     | 2.39                     | 0.58              |
| 36:BB:105:A:P     | 58:BZ:72:ARG:HH12  | 2.26                     | 0.58              |
| 36:BB:88:C:H2'    | 36:BB:89:G:C8      | 2.38                     | 0.58              |
| 44:BK:77:LEU:HD12 | 44:BK:107:ILE:CG2  | 2.32                     | 0.58              |
| 46:BN:18:ALA:CB   | 46:BN:21:LYS:HB2   | 2.33                     | 0.58              |
| 49:BQ:108:GLY:O   | 49:BQ:109:VAL:HG23 | 2.03                     | 0.58              |
| 53:BU:92:ARG:NH2  | 54:BV:11:GLN:H     | 2.01                     | 0.58              |
| 1:CA:1404:C:H5'   | 1:CA:1405:G:OP2    | 2.03                     | 0.58              |
| 1:CA:1441:G:H4'   | 1:CA:1442:G:C5     | 2.37                     | 0.58              |
| 1:CA:296:U:O2'    | 1:CA:297:G:H5'     | 2.03                     | 0.58              |
| 1:CA:992:U:H4'    | 1:CA:993:G:O5'     | 2.04                     | 0.58              |
| 1:CA:999:C:H2'    | 1:CA:1000:U:C6     | 2.39                     | 0.58              |
| 3:CC:25:GLY:O     | 3:CC:27:LYS:N      | 2.35                     | 0.58              |
| 3:CC:51:GLY:O     | 3:CC:115:LEU:HD21  | 2.03                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:CD:26:CYS:HA     | 4:CD:31:CYS:HA     | 1.85                     | 0.58              |
| 10:CJ:90:LEU:N     | 10:CJ:91:PRO:HD3   | 2.18                     | 0.58              |
| 24:CY:175:SER:O    | 24:CY:188:TYR:HD2  | 1.86                     | 0.58              |
| 24:CY:592:GLU:O    | 24:CY:592:GLU:HG2  | 2.04                     | 0.58              |
| 24:CY:628:ARG:HG2  | 24:CY:628:ARG:HH11 | 1.67                     | 0.58              |
| 33:D8:14:VAL:CG2   | 33:D8:22:VAL:HG13  | 2.32                     | 0.58              |
| 33:D8:16:ILE:HD12  | 33:D8:57:ARG:HG2   | 1.84                     | 0.58              |
| 35:DA:1301:A:O2'   | 35:DA:1302:A:C2'   | 2.47                     | 0.58              |
| 35:DA:1516:C:C2'   | 35:DA:1517:G:H5''  | 2.34                     | 0.58              |
| 35:DA:198:C:H42    | 35:DA:248:G:H1     | 1.50                     | 0.58              |
| 35:DA:320:A:H4'    | 35:DA:322:A:C8     | 2.38                     | 0.58              |
| 35:DA:448:U:O4     | 35:DA:583:G:H1'    | 2.03                     | 0.58              |
| 42:DH:105:LEU:HD23 | 42:DH:113:VAL:HB   | 1.85                     | 0.58              |
| 42:DH:86:GLU:HB2   | 42:DH:132:ARG:HB3  | 1.86                     | 0.58              |
| 46:DN:126:PRO:O    | 46:DN:127:ASP:HB2  | 2.03                     | 0.58              |
| 47:DO:114:ILE:HD12 | 47:DO:114:ILE:N    | 2.17                     | 0.58              |
| 51:DS:51:ALA:HB3   | 51:DS:73:LEU:HD12  | 1.85                     | 0.58              |
| 58:DZ:120:ILE:HB   | 58:DZ:171:ILE:O    | 2.03                     | 0.58              |
| 1:AA:393:A:O2'     | 1:AA:394:G:H5'     | 2.03                     | 0.58              |
| 1:AA:630:G:O2'     | 1:AA:631:G:H5''    | 2.03                     | 0.58              |
| 2:AB:8:LYS:O       | 2:AB:11:LEU:N      | 2.36                     | 0.58              |
| 2:AB:223:ILE:HG23  | 2:AB:226:ARG:NH1   | 2.18                     | 0.58              |
| 12:AL:28:LYS:HE2   | 12:AL:33:ARG:HH12  | 1.68                     | 0.58              |
| 12:AL:47:LYS:HD2   | 12:AL:48:PRO:HD3   | 1.85                     | 0.58              |
| 13:AM:15:VAL:HG12  | 13:AM:45:VAL:CG2   | 2.33                     | 0.58              |
| 13:AM:90:LEU:O     | 13:AM:91:ARG:C     | 2.40                     | 0.58              |
| 14:AN:37:PHE:HE1   | 14:AN:53:LEU:HD22  | 1.68                     | 0.58              |
| 19:AS:21:GLU:HG3   | 19:AS:22:LEU:HD23  | 1.84                     | 0.58              |
| 20:AT:73:HIS:O     | 20:AT:76:ALA:HB3   | 2.03                     | 0.58              |
| 7:AG:82:GLY:HA3    | 23:AX:13:A:H2      | 1.69                     | 0.58              |
| 24:AY:273:LEU:O    | 24:AY:276:VAL:HB   | 2.04                     | 0.58              |
| 24:AY:388:THR:HG23 | 24:AY:399:LEU:HD22 | 1.85                     | 0.58              |
| 24:AY:431:LEU:CD2  | 24:AY:466:LEU:HD13 | 2.33                     | 0.58              |
| 24:AY:65:ILE:O     | 24:AY:65:ILE:HG12  | 2.02                     | 0.58              |
| 25:B0:43:THR:O     | 25:B0:43:THR:HG23  | 2.03                     | 0.58              |
| 25:B0:51:VAL:CG2   | 25:B0:81:VAL:HG23  | 2.34                     | 0.58              |
| 31:B6:15:GLU:CG    | 31:B6:47:THR:HG21  | 2.33                     | 0.58              |
| 34:B9:10:ILE:O     | 34:B9:11:CYS:HB3   | 2.04                     | 0.58              |
| 35:BA:1662:C:H2'   | 35:BA:1663:C:C6    | 2.39                     | 0.58              |
| 35:BA:2260:C:H2'   | 35:BA:2261:C:H6    | 1.67                     | 0.58              |
| 35:BA:2329:G:H2'   | 35:BA:2330:G:H8    | 1.68                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:2572:A:H5'   | 35:BA:2574:G:C4'   | 2.28                     | 0.58              |
| 35:BA:2662:A:H2'   | 35:BA:2663:G:O4'   | 2.03                     | 0.58              |
| 35:BA:2762:G:H8    | 35:BA:2762:G:H5'   | 1.69                     | 0.58              |
| 38:BD:131:LEU:HD13 | 38:BD:136:ILE:HD11 | 1.86                     | 0.58              |
| 35:BA:2511:U:O3'   | 39:BE:123:ALA:HB3  | 2.04                     | 0.58              |
| 47:BO:47:ILE:CG2   | 47:BO:48:PRO:HD2   | 2.34                     | 0.58              |
| 51:BS:59:LYS:HG2   | 51:BS:60:GLY:N     | 2.18                     | 0.58              |
| 52:BT:83:ILE:HG13  | 52:BT:84:GLN:H     | 1.67                     | 0.58              |
| 54:BV:64:HIS:ND1   | 54:BV:92:THR:HG22  | 2.18                     | 0.58              |
| 57:BY:94:LYS:HG3   | 57:BY:102:CYS:SG   | 2.43                     | 0.58              |
| 57:BY:17:SER:OG    | 57:BY:18:GLY:N     | 2.36                     | 0.58              |
| 4:CD:17:VAL:HG12   | 4:CD:17:VAL:O      | 2.03                     | 0.58              |
| 13:CM:74:VAL:O     | 13:CM:77:ASN:HB2   | 2.02                     | 0.58              |
| 15:CO:76:GLU:C     | 15:CO:78:TYR:H     | 2.07                     | 0.58              |
| 17:CQ:76:LEU:HD12  | 17:CQ:77:VAL:N     | 2.19                     | 0.58              |
| 22:CV:5:G:O2'      | 22:CV:6:G:H5'      | 2.02                     | 0.58              |
| 7:CG:82:GLY:HA3    | 23:CX:13:A:H2      | 1.69                     | 0.58              |
| 24:CY:174:PHE:HZ   | 24:CY:261:GLY:HA2  | 1.66                     | 0.58              |
| 24:CY:259:PHE:HB2  | 24:CY:272:LEU:HD13 | 1.85                     | 0.58              |
| 24:CY:448:GLN:HG3  | 24:CY:448:GLN:O    | 2.04                     | 0.58              |
| 27:D2:20:GLU:HG3   | 27:D2:21:LEU:N     | 2.18                     | 0.58              |
| 30:D5:3:LYS:NZ     | 35:DA:2613:U:C2'   | 2.67                     | 0.58              |
| 33:D8:48:PHE:C     | 33:D8:49:VAL:HG22  | 2.23                     | 0.58              |
| 33:D8:51:ALA:N     | 33:D8:53:PRO:HD2   | 2.18                     | 0.58              |
| 35:DA:2115:G:N3    | 35:DA:2117:A:N7    | 2.52                     | 0.58              |
| 35:DA:2307:G:C2    | 35:DA:2308:G:H5''  | 2.38                     | 0.58              |
| 35:DA:2348:U:H2'   | 35:DA:2349:G:H5''  | 1.85                     | 0.58              |
| 35:DA:2461:C:H42   | 35:DA:2489:G:H1    | 1.51                     | 0.58              |
| 29:D4:3:GLU:HG2    | 36:DB:40:U:C5      | 2.39                     | 0.58              |
| 38:DD:34:VAL:C     | 38:DD:36:PRO:HD2   | 2.24                     | 0.58              |
| 38:DD:61:LEU:HB3   | 38:DD:63:ARG:HH12  | 1.69                     | 0.58              |
| 39:DE:45:THR:O     | 39:DE:46:ALA:HB2   | 2.03                     | 0.58              |
| 46:DN:18:ALA:CB    | 46:DN:21:LYS:HB2   | 2.33                     | 0.58              |
| 52:DT:129:ARG:O    | 52:DT:129:ARG:CG   | 2.51                     | 0.58              |
| 52:DT:11:GLU:C     | 52:DT:13:ARG:H     | 2.06                     | 0.58              |
| 52:DT:28:VAL:HG22  | 52:DT:47:GLY:H     | 1.69                     | 0.58              |
| 54:DV:81:TYR:C     | 54:DV:82:ARG:HD2   | 2.24                     | 0.58              |
| 56:DX:35:THR:HG22  | 56:DX:37:THR:N     | 2.11                     | 0.58              |
| 57:DY:39:VAL:HG12  | 57:DY:40:GLU:HG2   | 1.85                     | 0.58              |
| 58:DZ:125:LEU:HD23 | 58:DZ:164:ALA:O    | 2.04                     | 0.58              |
| 58:DZ:44:PHE:O     | 58:DZ:48:PHE:N     | 2.27                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1004:A:H61    | 1:AA:1034:G:C2'    | 2.14                     | 0.58              |
| 1:AA:925:G:H5'     | 1:AA:926:G:OP1     | 2.03                     | 0.58              |
| 3:AC:86:VAL:O      | 3:AC:90:GLU:HG2    | 2.04                     | 0.58              |
| 9:AI:47:LEU:C      | 9:AI:49:PRO:HD2    | 2.24                     | 0.58              |
| 1:AA:1124:G:H5'    | 10:AJ:35:SER:HB2   | 1.86                     | 0.58              |
| 10:AJ:78:ASN:HB2   | 10:AJ:81:THR:HG23  | 1.85                     | 0.58              |
| 15:AO:65:ARG:HH11  | 15:AO:65:ARG:HG2   | 1.67                     | 0.58              |
| 20:AT:88:VAL:O     | 20:AT:92:LEU:HG    | 2.04                     | 0.58              |
| 24:AY:25:LYS:HB2   | 62:AY:703:GDP:O2B  | 2.04                     | 0.58              |
| 24:AY:441:SER:O    | 24:AY:449:THR:HG23 | 2.02                     | 0.58              |
| 25:B0:73:GLY:C     | 25:B0:75:LEU:H     | 2.06                     | 0.58              |
| 27:B2:16:LEU:O     | 27:B2:20:GLU:HB3   | 2.04                     | 0.58              |
| 30:B5:48:GLU:O     | 30:B5:49:CYS:SG    | 2.62                     | 0.58              |
| 31:B6:8:LYS:HE3    | 31:B6:25:LYS:CD    | 2.29                     | 0.58              |
| 34:B9:22:ARG:HB2   | 34:B9:24:TYR:HE1   | 1.68                     | 0.58              |
| 35:BA:1308:A:H2'   | 35:BA:1309:G:O4'   | 2.02                     | 0.58              |
| 35:BA:1907:G:O2'   | 35:BA:1908:C:H5'   | 2.03                     | 0.58              |
| 31:B6:54:ILE:CD1   | 35:BA:2420:C:H5'   | 2.33                     | 0.58              |
| 35:BA:2603:G:O2'   | 35:BA:2604:U:H5'   | 2.04                     | 0.58              |
| 35:BA:651:G:H2'    | 35:BA:652:C:H5'    | 1.85                     | 0.58              |
| 35:BA:78:A:O2'     | 35:BA:79:G:H5'     | 2.03                     | 0.58              |
| 36:BB:87:G:H1      | 36:BB:91:C:H42     | 1.51                     | 0.58              |
| 35:BA:1059:G:H4'   | 44:BK:115:LEU:HD23 | 1.86                     | 0.58              |
| 46:BN:46:VAL:O     | 46:BN:47:ALA:HB3   | 2.02                     | 0.58              |
| 46:BN:87:LEU:HD21  | 46:BN:98:VAL:HG13  | 1.85                     | 0.58              |
| 47:BO:60:ALA:HA    | 47:BO:87:ILE:CD1   | 2.33                     | 0.58              |
| 52:BT:125:ARG:HH11 | 52:BT:125:ARG:CA   | 2.11                     | 0.58              |
| 2:CB:61:LEU:HD23   | 2:CB:68:ILE:HD11   | 1.85                     | 0.58              |
| 5:CE:60:TYR:CE1    | 5:CE:64:ARG:NH2    | 2.71                     | 0.58              |
| 6:CF:4:TYR:HE1     | 6:CF:92:LYS:HD2    | 1.69                     | 0.58              |
| 8:CH:12:ARG:NH1    | 8:CH:27:PRO:HD3    | 2.19                     | 0.58              |
| 10:CJ:32:ALA:HB3   | 10:CJ:78:ASN:HD21  | 1.67                     | 0.58              |
| 10:CJ:71:LEU:HD12  | 10:CJ:72:VAL:N     | 2.19                     | 0.58              |
| 11:CK:21:ILE:HD12  | 11:CK:21:ILE:N     | 2.18                     | 0.58              |
| 12:CL:53:ARG:NH1   | 12:CL:92:ASP:OD2   | 2.36                     | 0.58              |
| 19:CS:33:THR:HG22  | 19:CS:49:ILE:HG22  | 1.86                     | 0.58              |
| 24:CY:224:ASP:OD2  | 24:CY:245:ALA:HB2  | 2.03                     | 0.58              |
| 28:D3:52:HIS:H     | 28:D3:52:HIS:CD2   | 2.19                     | 0.58              |
| 30:D5:48:GLU:O     | 30:D5:49:CYS:CB    | 2.50                     | 0.58              |
| 35:DA:1405:U:H2'   | 35:DA:1406:U:C6    | 2.38                     | 0.58              |
| 35:DA:200:U:H2'    | 35:DA:201:C:H5'    | 1.85                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:D0:43:THR:HG22  | 35:DA:2331:G:O2'   | 2.04                     | 0.58              |
| 35:DA:2577:A:C5'   | 35:DA:2578:G:H5'   | 2.33                     | 0.58              |
| 30:D5:43:HIS:HD2   | 35:DA:2815:C:O2'   | 1.86                     | 0.58              |
| 35:DA:292:C:O2'    | 35:DA:293:U:H5'    | 2.03                     | 0.58              |
| 35:DA:680:G:H2'    | 35:DA:681:G:C8     | 2.38                     | 0.58              |
| 35:DA:946:G:H2'    | 35:DA:947:G:C8     | 2.38                     | 0.58              |
| 35:DA:996:A:O3'    | 53:DU:92:ARG:HG2   | 2.04                     | 0.58              |
| 37:DC:138:LEU:HD22 | 37:DC:139:PRO:HD2  | 1.85                     | 0.58              |
| 38:DD:26:LYS:O     | 38:DD:27:THR:HG22  | 2.03                     | 0.58              |
| 40:DF:28:ILE:HG21  | 40:DF:116:ASP:HB2  | 1.85                     | 0.58              |
| 1:AA:264:U:O2'     | 17:AQ:64:PRO:HB2   | 2.04                     | 0.58              |
| 1:AA:45:U:H2'      | 1:AA:46:G:C8       | 2.38                     | 0.58              |
| 9:AI:126:SER:O     | 9:AI:128:ARG:HD2   | 2.03                     | 0.58              |
| 19:AS:78:ARG:HB2   | 19:AS:81:ARG:NH1   | 2.18                     | 0.58              |
| 19:AS:9:VAL:O      | 19:AS:9:VAL:CG1    | 2.52                     | 0.58              |
| 24:AY:314:PHE:HD1  | 24:AY:315:LYS:HB2  | 1.68                     | 0.58              |
| 24:AY:468:ARG:C    | 24:AY:470:PHE:H    | 2.07                     | 0.58              |
| 33:B8:10:ALA:O     | 33:B8:14:VAL:HG12  | 2.04                     | 0.58              |
| 35:BA:1638:C:H2'   | 35:BA:1639:U:O4'   | 2.02                     | 0.58              |
| 35:BA:572:A:C2     | 35:BA:2033:A:C2    | 2.92                     | 0.58              |
| 36:BB:91:C:O2'     | 36:BB:92:C:H5'     | 2.03                     | 0.58              |
| 38:BD:147:LEU:HD13 | 38:BD:155:LEU:CD1  | 2.33                     | 0.58              |
| 39:BE:77:ILE:HG22  | 39:BE:78:LEU:CD1   | 2.34                     | 0.58              |
| 40:BF:18:ARG:HG2   | 40:BF:19:GLU:N     | 2.19                     | 0.58              |
| 58:BZ:153:SER:C    | 58:BZ:155:LEU:HD23 | 2.24                     | 0.58              |
| 1:CA:1117:G:H5'    | 1:CA:1117:G:H8     | 1.68                     | 0.58              |
| 1:CA:191:G:H1'     | 20:CT:105:SER:HA   | 1.85                     | 0.58              |
| 3:CC:112:SER:HB3   | 3:CC:115:LEU:HD12  | 1.84                     | 0.58              |
| 3:CC:130:VAL:HG21  | 3:CC:157:ILE:HG23  | 1.86                     | 0.58              |
| 9:CI:79:LEU:CD1    | 9:CI:83:ARG:HD2    | 2.34                     | 0.58              |
| 24:CY:637:ARG:HH11 | 24:CY:637:ARG:HG3  | 1.69                     | 0.58              |
| 35:DA:2629:A:N3    | 35:DA:2629:A:H2'   | 2.18                     | 0.58              |
| 35:DA:2742:C:C2'   | 35:DA:2743:C:H5'   | 2.33                     | 0.58              |
| 32:D7:4:THR:HB     | 35:DA:788:A:O2'    | 2.03                     | 0.58              |
| 36:DB:112:U:H2'    | 36:DB:113:G:C8     | 2.35                     | 0.58              |
| 39:DE:34:VAL:HG11  | 39:DE:78:LEU:HD22  | 1.84                     | 0.58              |
| 40:DF:163:VAL:O    | 40:DF:166:ALA:HB3  | 2.04                     | 0.58              |
| 46:DN:102:ALA:O    | 46:DN:106:MET:HE2  | 2.03                     | 0.58              |
| 35:DA:1242:A:C6    | 48:DP:8:PRO:HG2    | 2.39                     | 0.58              |
| 50:DR:12:ARG:HH11  | 50:DR:12:ARG:HG3   | 1.69                     | 0.58              |
| 53:DU:83:LEU:HD12  | 53:DU:83:LEU:N     | 2.18                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 54:DV:64:HIS:ND1  | 54:DV:92:THR:HG22  | 2.19                     | 0.58              |
| 55:DW:59:VAL:CG1  | 55:DW:59:VAL:O     | 2.51                     | 0.58              |
| 57:DY:61:ILE:HG12 | 57:DY:62:GLU:N     | 2.19                     | 0.58              |
| 1:AA:1258:G:O2'   | 1:AA:1259:C:H5'    | 2.04                     | 0.58              |
| 1:AA:1303:C:C2'   | 1:AA:1304:G:H5'    | 2.34                     | 0.58              |
| 1:AA:1346:A:N6    | 1:AA:1374:A:H3'    | 2.19                     | 0.58              |
| 1:AA:513:C:O2'    | 1:AA:514:C:H5'     | 2.04                     | 0.58              |
| 2:AB:30:ARG:HG3   | 2:AB:31:TYR:CD2    | 2.38                     | 0.58              |
| 10:AJ:18:ALA:O    | 10:AJ:20:ALA:N     | 2.37                     | 0.58              |
| 13:AM:49:THR:HB   | 13:AM:52:GLU:HG3   | 1.85                     | 0.58              |
| 24:AY:225:GLU:O   | 24:AY:228:MET:HB3  | 2.04                     | 0.58              |
| 24:AY:438:PHE:HB2 | 24:AY:452:SER:O    | 2.04                     | 0.58              |
| 25:B0:49:LYS:O    | 25:B0:51:VAL:HG23  | 2.04                     | 0.58              |
| 33:B8:25:MET:O    | 33:B8:47:LYS:HG2   | 2.03                     | 0.58              |
| 33:B8:50:LEU:O    | 33:B8:52:LYS:N     | 2.33                     | 0.58              |
| 35:BA:1043:C:C3'  | 35:BA:1044:G:H5''  | 2.34                     | 0.58              |
| 35:BA:1668:A:N6   | 35:BA:1676:A:H61   | 2.01                     | 0.58              |
| 35:BA:1794:U:O2'  | 35:BA:1795:C:H5'   | 2.03                     | 0.58              |
| 35:BA:2097:C:H2'  | 35:BA:2098:U:H6    | 1.68                     | 0.58              |
| 35:BA:2629:A:N3   | 35:BA:2629:A:H2'   | 2.17                     | 0.58              |
| 35:BA:2649:U:O2'  | 35:BA:2650:U:H5'   | 2.04                     | 0.58              |
| 35:BA:2815:C:H2'  | 35:BA:2816:C:H6    | 1.68                     | 0.58              |
| 35:BA:448:U:O4    | 35:BA:583:G:H1'    | 2.03                     | 0.58              |
| 35:BA:529:A:H4'   | 35:BA:530:G:O5'    | 2.04                     | 0.58              |
| 38:BD:131:LEU:N   | 38:BD:131:LEU:CD1  | 2.67                     | 0.58              |
| 38:BD:259:THR:O   | 38:BD:260:ARG:C    | 2.41                     | 0.58              |
| 39:BE:144:ARG:O   | 39:BE:145:LYS:O    | 2.21                     | 0.58              |
| 40:BF:6:VAL:H     | 40:BF:125:LEU:HD21 | 1.69                     | 0.58              |
| 42:BH:28:GLY:HA3  | 42:BH:79:VAL:CG2   | 2.34                     | 0.58              |
| 46:BN:102:ALA:O   | 46:BN:106:MET:HE2  | 2.04                     | 0.58              |
| 48:BP:83:VAL:H    | 48:BP:115:LEU:HD21 | 1.69                     | 0.58              |
| 52:BT:26:ASP:OD2  | 52:BT:26:ASP:C     | 2.42                     | 0.58              |
| 55:BW:17:VAL:O    | 55:BW:20:VAL:HG22  | 2.04                     | 0.58              |
| 57:BY:17:SER:HB2  | 57:BY:71:LYS:HD2   | 1.85                     | 0.58              |
| 58:BZ:144:LEU:N   | 58:BZ:144:LEU:HD22 | 2.19                     | 0.58              |
| 1:CA:405:U:H3'    | 1:CA:406:G:H5'     | 1.85                     | 0.58              |
| 1:CA:52:G:O2'     | 1:CA:53:A:H5'      | 2.03                     | 0.58              |
| 1:CA:630:G:C2'    | 1:CA:631:G:C5'     | 2.81                     | 0.58              |
| 6:CF:37:VAL:HG12  | 6:CF:38:GLU:O      | 2.04                     | 0.58              |
| 6:CF:33:TYR:HA    | 6:CF:71:ARG:HH21   | 1.69                     | 0.58              |
| 8:CH:89:PRO:HA    | 8:CH:92:ARG:HH11   | 1.69                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:CI:47:LEU:C      | 9:CI:49:PRO:HD2    | 2.24                     | 0.58              |
| 11:CK:67:ASP:OD1   | 11:CK:71:LYS:HE3   | 2.04                     | 0.58              |
| 21:CU:6:ARG:NH2    | 21:CU:15:ARG:NH2   | 2.51                     | 0.58              |
| 24:CY:17:ILE:H     | 24:CY:17:ILE:CD1   | 2.16                     | 0.58              |
| 24:CY:36:THR:HB    | 24:CY:72:CYS:HB2   | 1.85                     | 0.58              |
| 25:D0:43:THR:O     | 25:D0:43:THR:HG23  | 2.03                     | 0.58              |
| 30:D5:36:CYS:SG    | 30:D5:49:CYS:SG    | 3.01                     | 0.58              |
| 35:DA:1516:C:O2'   | 35:DA:1517:G:H5''  | 2.03                     | 0.58              |
| 35:DA:1578:U:C2'   | 35:DA:1579:A:H5''  | 2.32                     | 0.58              |
| 35:DA:175:G:O2'    | 35:DA:176:G:H5'    | 2.03                     | 0.58              |
| 35:DA:206:U:O2     | 35:DA:206:U:H2'    | 2.03                     | 0.58              |
| 35:DA:2097:C:H2'   | 35:DA:2098:U:C6    | 2.38                     | 0.58              |
| 35:DA:2745:C:H2'   | 35:DA:2746:U:C6    | 2.39                     | 0.58              |
| 35:DA:787:U:OP1    | 35:DA:1780:A:N6    | 2.37                     | 0.58              |
| 35:DA:850:C:O2'    | 35:DA:851:U:H5'    | 2.03                     | 0.58              |
| 36:DB:115:G:H2'    | 36:DB:116:G:H8     | 1.68                     | 0.58              |
| 35:DA:2170:A:H5''  | 37:DC:135:ARG:HH21 | 1.67                     | 0.58              |
| 39:DE:52:LEU:O     | 39:DE:74:PRO:HA    | 2.03                     | 0.58              |
| 40:DF:40:GLN:OE1   | 40:DF:184:TYR:HB2  | 2.04                     | 0.58              |
| 48:DP:97:PRO:HD3   | 48:DP:126:VAL:O    | 2.04                     | 0.58              |
| 48:DP:30:THR:O     | 48:DP:33:ARG:N     | 2.26                     | 0.58              |
| 48:DP:91:PHE:CE2   | 48:DP:95:VAL:HG12  | 2.38                     | 0.58              |
| 49:DQ:39:PRO:HB3   | 49:DQ:99:PRO:HD3   | 1.86                     | 0.58              |
| 50:DR:99:LYS:N     | 50:DR:99:LYS:CD    | 2.58                     | 0.58              |
| 57:DY:88:LYS:HD2   | 57:DY:88:LYS:N     | 2.19                     | 0.58              |
| 58:DZ:155:LEU:HD23 | 58:DZ:155:LEU:N    | 2.18                     | 0.58              |
| 1:AA:1144:G:H21    | 1:AA:1146:A:H62    | 1.51                     | 0.58              |
| 1:AA:960:U:C5      | 1:AA:1225:A:C8     | 2.92                     | 0.58              |
| 1:AA:992:U:H4'     | 1:AA:993:G:O5'     | 2.04                     | 0.58              |
| 5:AE:144:THR:O     | 5:AE:148:VAL:HG23  | 2.03                     | 0.58              |
| 6:AF:69:GLU:O      | 6:AF:72:VAL:HG12   | 2.04                     | 0.58              |
| 8:AH:6:ILE:N       | 8:AH:6:ILE:HD12    | 2.19                     | 0.58              |
| 8:AH:20:TYR:CE1    | 8:AH:76:PRO:HG2    | 2.39                     | 0.58              |
| 10:AJ:55:LYS:H     | 10:AJ:55:LYS:HE3   | 1.67                     | 0.58              |
| 19:AS:31:ILE:HG23  | 19:AS:49:ILE:HG23  | 1.86                     | 0.58              |
| 24:AY:605:ILE:CD1  | 24:AY:677:GLN:HG2  | 2.34                     | 0.58              |
| 24:AY:632:LEU:HD12 | 24:AY:645:ALA:HA   | 1.85                     | 0.58              |
| 26:B1:80:LEU:CD2   | 26:B1:81:LYS:N     | 2.66                     | 0.58              |
| 31:B6:35:GLU:HB3   | 31:B6:51:GLU:HB2   | 1.86                     | 0.58              |
| 31:B6:51:GLU:HG2   | 31:B6:52:VAL:H     | 1.67                     | 0.58              |
| 35:BA:2297:C:O2'   | 35:BA:2298:A:H5'   | 2.04                     | 0.58              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:2453:A:H2'   | 35:BA:2454:G:H8    | 1.69                     | 0.58              |
| 35:BA:621:A:H2'    | 35:BA:622:G:C5'    | 2.31                     | 0.58              |
| 35:BA:784:A:H5''   | 38:BD:227:ASN:ND2  | 2.19                     | 0.58              |
| 35:BA:848:G:C2     | 35:BA:933:A:H1'    | 2.39                     | 0.58              |
| 35:BA:2122:U:H1'   | 37:BC:167:ASP:OD2  | 2.04                     | 0.58              |
| 39:BE:64:LYS:C     | 39:BE:66:HIS:H     | 2.07                     | 0.58              |
| 40:BF:158:THR:HG21 | 40:BF:163:VAL:HB   | 1.86                     | 0.58              |
| 35:BA:443:A:H3'    | 40:BF:45:ARG:HH21  | 1.68                     | 0.58              |
| 41:BG:119:GLY:HA3  | 41:BG:181:ARG:H    | 1.69                     | 0.58              |
| 41:BG:141:PHE:O    | 41:BG:144:ILE:HG22 | 2.04                     | 0.58              |
| 44:BK:7:VAL:O      | 44:BK:7:VAL:CG1    | 2.46                     | 0.58              |
| 45:BL:90:UNK:C     | 45:BL:92:UNK:H     | 2.16                     | 0.58              |
| 48:BP:84:ASN:C     | 48:BP:86:LYS:N     | 2.57                     | 0.58              |
| 50:BR:10:LEU:HD22  | 50:BR:17:ARG:CD    | 2.33                     | 0.58              |
| 57:BY:8:LYS:HE2    | 57:BY:72:VAL:HG23  | 1.85                     | 0.58              |
| 1:CA:1410:G:H1     | 1:CA:1490:C:H42    | 1.52                     | 0.58              |
| 1:CA:1456:G:H2'    | 1:CA:1457:G:H5'    | 1.85                     | 0.58              |
| 24:CY:119:GLU:C    | 24:CY:120:THR:HG1  | 2.07                     | 0.58              |
| 24:CY:212:TYR:HA   | 24:CY:215:LYS:HD2  | 1.84                     | 0.58              |
| 24:CY:296:GLY:O    | 24:CY:297:GLU:HB3  | 2.04                     | 0.58              |
| 24:CY:415:PRO:HA   | 24:CY:474:ALA:HB2  | 1.84                     | 0.58              |
| 25:D0:51:VAL:HG21  | 25:D0:79:VAL:O     | 2.03                     | 0.58              |
| 29:D4:27:THR:O     | 29:D4:28:LYS:HB3   | 2.02                     | 0.58              |
| 35:DA:1068:G:N2    | 35:DA:1096:A:H5'   | 2.19                     | 0.58              |
| 35:DA:2647:U:H2'   | 35:DA:2648:C:C6    | 2.39                     | 0.58              |
| 35:DA:529:A:H4'    | 35:DA:530:G:O5'    | 2.04                     | 0.58              |
| 35:DA:624:C:H41    | 48:DP:107:LYS:HZ3  | 1.51                     | 0.58              |
| 36:DB:20:C:H2'     | 36:DB:21:G:H5'     | 1.85                     | 0.58              |
| 39:DE:64:LYS:C     | 39:DE:66:HIS:H     | 2.06                     | 0.58              |
| 42:DH:136:ILE:HD12 | 42:DH:136:ILE:N    | 2.19                     | 0.58              |
| 48:DP:135:LEU:HD13 | 48:DP:135:LEU:O    | 2.03                     | 0.58              |
| 48:DP:84:ASN:C     | 48:DP:86:LYS:H     | 2.05                     | 0.58              |
| 53:DU:26:GLY:O     | 53:DU:28:ARG:N     | 2.37                     | 0.58              |
| 58:DZ:149:SER:HB2  | 58:DZ:172:ALA:O    | 2.04                     | 0.58              |
| 58:DZ:17:ALA:HA    | 58:DZ:20:ARG:HG2   | 1.85                     | 0.58              |
| 1:AA:122:G:O2'     | 1:AA:123:C:H5'     | 2.04                     | 0.57              |
| 1:AA:1392:G:N2     | 1:AA:1502:A:H8     | 2.01                     | 0.57              |
| 1:AA:1442:G:C5     | 1:AA:1442(B):A:H2  | 2.21                     | 0.57              |
| 1:AA:677:U:H3      | 1:AA:713:G:H22     | 1.50                     | 0.57              |
| 2:AB:220:ASP:O     | 2:AB:223:ILE:N     | 2.35                     | 0.57              |
| 2:AB:24:TRP:CZ3    | 2:AB:26:PRO:HA     | 2.39                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:AD:114:ARG:HG3   | 4:AD:114:ARG:NH1   | 2.18                     | 0.57              |
| 5:AE:101:ILE:CD1   | 5:AE:119:LEU:HA    | 2.26                     | 0.57              |
| 9:AI:114:TYR:HE1   | 10:AJ:60:ARG:N     | 1.97                     | 0.57              |
| 22:AW:7:G:H3'      | 22:AW:8:U:C5'      | 2.30                     | 0.57              |
| 26:B1:5:CYS:O      | 26:B1:9:GLY:HA2    | 2.03                     | 0.57              |
| 29:B4:25:TYR:O     | 29:B4:26:SER:HB3   | 2.03                     | 0.57              |
| 30:B5:3:LYS:HZ2    | 30:B5:5:PRO:HB2    | 1.69                     | 0.57              |
| 33:B8:14:VAL:CG2   | 33:B8:22:VAL:HG13  | 2.34                     | 0.57              |
| 35:BA:120:U:H5'    | 35:BA:121:G:OP1    | 2.03                     | 0.57              |
| 35:BA:1717:G:C2'   | 35:BA:1718:G:H5''  | 2.34                     | 0.57              |
| 37:BC:57:GLN:HE21  | 37:BC:205:ALA:HA   | 1.68                     | 0.57              |
| 39:BE:111:ARG:HA   | 50:BR:2:ARG:CB     | 2.29                     | 0.57              |
| 40:BF:9:ILE:HG23   | 40:BF:13:SER:O     | 2.03                     | 0.57              |
| 41:BG:180:PHE:O    | 41:BG:181:ARG:C    | 2.41                     | 0.57              |
| 45:BL:113:UNK:HA   | 45:BL:117:UNK:O    | 2.03                     | 0.57              |
| 51:BS:34:HIS:NE2   | 51:BS:54:LEU:HB3   | 2.19                     | 0.57              |
| 52:BT:55:ASN:N     | 52:BT:59:THR:CG2   | 2.66                     | 0.57              |
| 57:BY:17:SER:CB    | 57:BY:71:LYS:HD2   | 2.34                     | 0.57              |
| 58:BZ:29:TYR:CB    | 58:BZ:34:ASN:HB2   | 2.33                     | 0.57              |
| 1:CA:1375:A:H5'    | 1:CA:1376:U:OP2    | 2.04                     | 0.57              |
| 2:CB:178:ARG:HB2   | 2:CB:178:ARG:HH11  | 1.68                     | 0.57              |
| 3:CC:181:ASN:HD21  | 3:CC:204:LEU:HD12  | 1.68                     | 0.57              |
| 3:CC:35:GLU:OE2    | 3:CC:59:ARG:NH1    | 2.37                     | 0.57              |
| 4:CD:57:ARG:HG2    | 4:CD:57:ARG:HH11   | 1.69                     | 0.57              |
| 5:CE:12:LEU:CD1    | 5:CE:31:LEU:HB3    | 2.34                     | 0.57              |
| 5:CE:33:VAL:HG12   | 5:CE:34:VAL:N      | 2.17                     | 0.57              |
| 6:CF:9:VAL:HB      | 6:CF:87:ARG:HB2    | 1.86                     | 0.57              |
| 15:CO:17:ARG:HD3   | 15:CO:26:GLU:HG3   | 1.85                     | 0.57              |
| 15:CO:74:ASP:C     | 15:CO:76:GLU:H     | 2.08                     | 0.57              |
| 17:CQ:53:LEU:HD21  | 17:CQ:85:VAL:HG11  | 1.85                     | 0.57              |
| 24:CY:156:ARG:HB2  | 24:CY:157:LEU:HD23 | 1.86                     | 0.57              |
| 24:CY:458:HIS:O    | 24:CY:461:ILE:HG13 | 2.02                     | 0.57              |
| 24:CY:614:GLU:HA   | 24:CY:617:MET:HB2  | 1.84                     | 0.57              |
| 24:CY:25:LYS:NZ    | 24:CY:86:GLY:HA2   | 2.19                     | 0.57              |
| 30:D5:43:HIS:CD2   | 35:DA:2815:C:O2'   | 2.56                     | 0.57              |
| 34:D9:34:GLN:O     | 34:D9:35:ARG:HB2   | 2.04                     | 0.57              |
| 35:DA:1473:G:H2'   | 35:DA:1474:C:O4'   | 2.04                     | 0.57              |
| 35:DA:1558:A:H4'   | 35:DA:1559:G:O5'   | 2.04                     | 0.57              |
| 35:DA:2556:C:H2'   | 35:DA:2557:G:O4'   | 2.04                     | 0.57              |
| 35:DA:271(U):G:O2' | 35:DA:271(V):G:H5' | 2.03                     | 0.57              |
| 38:DD:77:ALA:CB    | 38:DD:97:TYR:HA    | 2.34                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:DE:101:ARG:NE  | 39:DE:171:GLU:HB2 | 2.19                     | 0.57              |
| 39:DE:44:TYR:O    | 39:DE:45:THR:HB   | 2.04                     | 0.57              |
| 39:DE:47:VAL:CG1  | 39:DE:48:GLN:H    | 2.12                     | 0.57              |
| 48:DP:47:ASP:CB   | 48:DP:51:PHE:HB2  | 2.34                     | 0.57              |
| 51:DS:54:LEU:O    | 51:DS:54:LEU:HD13 | 2.03                     | 0.57              |
| 57:DY:12:THR:HG22 | 57:DY:75:ILE:HG21 | 1.86                     | 0.57              |
| 57:DY:91:GLU:O    | 57:DY:92:ASN:HB2  | 2.04                     | 0.57              |
| 58:DZ:109:ALA:C   | 58:DZ:111:VAL:H   | 2.05                     | 0.57              |
| 58:DZ:151:HIS:CB  | 58:DZ:170:THR:HA  | 2.33                     | 0.57              |
| 58:DZ:67:LEU:N    | 58:DZ:67:LEU:HD12 | 2.18                     | 0.57              |
| 1:AA:1270:C:H4'   | 1:AA:1313:U:O2'   | 2.03                     | 0.57              |
| 1:AA:1479:C:H2'   | 1:AA:1480:G:H8    | 1.69                     | 0.57              |
| 2:AB:235:SER:O    | 2:AB:237:ALA:N    | 2.31                     | 0.57              |
| 4:AD:104:VAL:HG21 | 4:AD:140:VAL:HG21 | 1.86                     | 0.57              |
| 4:AD:159:ARG:HH11 | 4:AD:159:ARG:HG3  | 1.68                     | 0.57              |
| 4:AD:162:LEU:CD1  | 4:AD:181:MET:HG2  | 2.34                     | 0.57              |
| 21:AU:6:ARG:NH2   | 21:AU:15:ARG:NH2  | 2.52                     | 0.57              |
| 13:AM:119:GLY:HA2 | 22:AV:29:G:OP1    | 2.03                     | 0.57              |
| 24:AY:112:GLN:O   | 24:AY:115:GLU:HB3 | 2.05                     | 0.57              |
| 24:AY:680:PRO:O   | 24:AY:682:GLN:N   | 2.33                     | 0.57              |
| 26:B1:6:GLU:OE1   | 26:B1:61:ARG:N    | 2.36                     | 0.57              |
| 32:B7:4:THR:HB    | 35:BA:788:A:O2'   | 2.03                     | 0.57              |
| 35:BA:1428:C:N4   | 35:BA:1569:A:H3'  | 2.19                     | 0.57              |
| 35:BA:16:G:H2'    | 35:BA:17:G:H8     | 1.68                     | 0.57              |
| 35:BA:1942:C:H3'  | 35:BA:1943:U:H5'' | 1.86                     | 0.57              |
| 35:BA:1943:U:H4'  | 35:BA:1944:U:OP1  | 2.03                     | 0.57              |
| 35:BA:2317:C:H2'  | 35:BA:2318:G:C5'  | 2.33                     | 0.57              |
| 35:BA:2377:A:H2'  | 35:BA:2378:A:C8   | 2.38                     | 0.57              |
| 41:BG:126:ASP:OD1 | 41:BG:130:ASN:HB2 | 2.04                     | 0.57              |
| 42:BH:19:VAL:O    | 42:BH:20:ALA:HB2  | 2.04                     | 0.57              |
| 44:BK:21:PRO:HA   | 44:BK:23:VAL:N    | 2.19                     | 0.57              |
| 48:BP:114:ILE:O   | 48:BP:130:PHE:HA  | 2.03                     | 0.57              |
| 54:BV:35:LEU:O    | 54:BV:37:VAL:N    | 2.36                     | 0.57              |
| 54:BV:81:TYR:C    | 54:BV:82:ARG:HD2  | 2.24                     | 0.57              |
| 1:CA:219:C:H2'    | 1:CA:220:G:O4'    | 2.03                     | 0.57              |
| 2:CB:223:ILE:HG23 | 2:CB:226:ARG:NH1  | 2.19                     | 0.57              |
| 3:CC:154:SER:O    | 3:CC:165:THR:HA   | 2.03                     | 0.57              |
| 4:CD:104:VAL:HG21 | 4:CD:140:VAL:HG21 | 1.85                     | 0.57              |
| 8:CH:104:ARG:HB3  | 8:CH:108:GLY:H    | 1.69                     | 0.57              |
| 8:CH:109:ILE:HG12 | 8:CH:110:ALA:H    | 1.68                     | 0.57              |
| 18:CR:58:LEU:HD12 | 18:CR:58:LEU:N    | 2.18                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:CW:25:U:O2'     | 22:CW:26:C:H5'     | 2.04                     | 0.57              |
| 24:CY:25:LYS:HZ3   | 24:CY:86:GLY:HA2   | 1.68                     | 0.57              |
| 31:D6:45:LYS:HG2   | 35:DA:2371:G:H5''  | 1.86                     | 0.57              |
| 32:D7:35:ARG:HG2   | 32:D7:35:ARG:HH11  | 1.69                     | 0.57              |
| 35:DA:1036:G:OP2   | 42:DH:59:ARG:NH1   | 2.37                     | 0.57              |
| 35:DA:1835:G:H1'   | 35:DA:1931:U:O2    | 2.04                     | 0.57              |
| 35:DA:2219:G:O2'   | 35:DA:2220:G:H5'   | 2.04                     | 0.57              |
| 36:DB:103:G:N2     | 58:DZ:73:GLN:HE22  | 1.95                     | 0.57              |
| 37:DC:4:HIS:ND1    | 37:DC:8:TYR:CE2    | 2.72                     | 0.57              |
| 40:DF:148:LEU:HD23 | 40:DF:191:ARG:NH1  | 2.19                     | 0.57              |
| 40:DF:6:VAL:H      | 40:DF:125:LEU:HD21 | 1.69                     | 0.57              |
| 41:DG:52:ILE:HG22  | 41:DG:54:GLU:H     | 1.69                     | 0.57              |
| 42:DH:148:ILE:O    | 42:DH:151:ILE:HG12 | 2.05                     | 0.57              |
| 46:DN:62:VAL:HG13  | 46:DN:62:VAL:O     | 2.03                     | 0.57              |
| 47:DO:26:LYS:HB3   | 47:DO:30:ALA:CB    | 2.35                     | 0.57              |
| 49:DQ:97:VAL:HG21  | 49:DQ:103:MET:HE3  | 1.85                     | 0.57              |
| 53:DU:70:ARG:HA    | 53:DU:74:LEU:O     | 2.04                     | 0.57              |
| 53:DU:92:ARG:NH2   | 54:DV:11:GLN:H     | 2.01                     | 0.57              |
| 57:DY:25:GLY:HA3   | 57:DY:39:VAL:CG1   | 2.34                     | 0.57              |
| 58:DZ:171:ILE:HG13 | 58:DZ:172:ALA:N    | 2.19                     | 0.57              |
| 1:AA:1370:G:C2     | 1:AA:1371:G:C8     | 2.93                     | 0.57              |
| 1:AA:833:U:H2'     | 1:AA:834:C:C6      | 2.39                     | 0.57              |
| 3:AC:134:ILE:HD11  | 3:AC:153:VAL:HG23  | 1.85                     | 0.57              |
| 4:AD:162:LEU:HD11  | 4:AD:181:MET:CG    | 2.35                     | 0.57              |
| 12:AL:53:ARG:NH1   | 12:AL:92:ASP:OD2   | 2.37                     | 0.57              |
| 13:AM:83:ASP:CG    | 13:AM:84:ILE:N     | 2.58                     | 0.57              |
| 22:AW:3:C:H2'      | 22:AW:4:G:H5''     | 1.85                     | 0.57              |
| 24:AY:496:LYS:HE2  | 24:AY:498:ILE:CD1  | 2.34                     | 0.57              |
| 25:B0:36:ILE:HG13  | 25:B0:36:ILE:O     | 2.04                     | 0.57              |
| 26:B1:76:ARG:NH2   | 26:B1:95:LEU:HD22  | 2.20                     | 0.57              |
| 28:B3:5:LYS:HE3    | 28:B3:34:GLU:OE1   | 2.04                     | 0.57              |
| 35:BA:1840:G:H1    | 35:BA:1902:C:H42   | 1.52                     | 0.57              |
| 35:BA:2011:U:H2'   | 35:BA:2012:G:H5'   | 1.87                     | 0.57              |
| 35:BA:207:A:H2'    | 35:BA:208:C:O4'    | 2.02                     | 0.57              |
| 35:BA:2115:G:N3    | 35:BA:2117:A:N7    | 2.52                     | 0.57              |
| 35:BA:2219:G:O2'   | 35:BA:2220:G:H5'   | 2.04                     | 0.57              |
| 35:BA:2312:U:H2'   | 35:BA:2313:C:C5'   | 2.34                     | 0.57              |
| 35:BA:2777:G:H5''  | 35:BA:2778:A:H5''  | 1.86                     | 0.57              |
| 35:BA:328:U:H4'    | 57:BY:68:HIS:CD2   | 2.39                     | 0.57              |
| 35:BA:810:U:OP1    | 35:BA:1253:A:N7    | 2.38                     | 0.57              |
| 36:BB:49:C:H2'     | 36:BB:50:G:C8      | 2.39                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:BC:191:ARG:HH11 | 37:BC:191:ARG:HG3  | 1.68                     | 0.57              |
| 40:BF:119:ARG:HH11 | 40:BF:119:ARG:HG2  | 1.69                     | 0.57              |
| 48:BP:91:PHE:HZ    | 48:BP:100:LEU:HD11 | 1.69                     | 0.57              |
| 51:BS:30:ARG:NH2   | 51:BS:62:LYS:HD2   | 2.19                     | 0.57              |
| 53:BU:49:HIS:HA    | 53:BU:52:ARG:HB2   | 1.85                     | 0.57              |
| 1:CA:1148:U:H2'    | 1:CA:1149:C:O4'    | 2.04                     | 0.57              |
| 1:CA:1366:C:H2'    | 1:CA:1367:C:H6     | 1.70                     | 0.57              |
| 1:CA:165:C:O2'     | 1:CA:166:G:H5'     | 2.04                     | 0.57              |
| 1:CA:662:G:H2'     | 1:CA:663:A:H8      | 1.67                     | 0.57              |
| 1:CA:977:A:H2'     | 1:CA:978:A:H5'     | 1.86                     | 0.57              |
| 3:CC:131:ARG:NH2   | 3:CC:168:ALA:HB2   | 2.20                     | 0.57              |
| 8:CH:20:TYR:CE1    | 8:CH:76:PRO:HG2    | 2.39                     | 0.57              |
| 9:CI:8:GLY:CA      | 9:CI:79:LEU:HD12   | 2.34                     | 0.57              |
| 16:CP:28:ARG:HH11  | 16:CP:28:ARG:HG2   | 1.70                     | 0.57              |
| 17:CQ:44:ALA:HA    | 17:CQ:71:PHE:O     | 2.03                     | 0.57              |
| 24:CY:355:LEU:HB3  | 24:CY:369:LEU:HD11 | 1.85                     | 0.57              |
| 24:CY:99:ARG:HE    | 24:CY:128:TYR:CB   | 2.16                     | 0.57              |
| 34:D9:17:ILE:HG22  | 34:D9:18:ARG:N     | 2.19                     | 0.57              |
| 35:DA:1247:A:OP1   | 40:DF:95:ARG:NH2   | 2.37                     | 0.57              |
| 31:D6:54:ILE:CD1   | 35:DA:2420:C:H5'   | 2.34                     | 0.57              |
| 30:D5:3:LYS:HZ1    | 35:DA:2613:U:C2'   | 2.17                     | 0.57              |
| 35:DA:321:G:C2     | 35:DA:341:G:H4'    | 2.39                     | 0.57              |
| 32:D7:33:ARG:NH1   | 35:DA:467:G:OP1    | 2.37                     | 0.57              |
| 36:DB:87:G:H1      | 36:DB:91:C:H42     | 1.52                     | 0.57              |
| 36:DB:88:C:H2'     | 36:DB:89:G:C8      | 2.39                     | 0.57              |
| 38:DD:145:VAL:HG12 | 38:DD:146:GLU:N    | 2.18                     | 0.57              |
| 35:DA:2511:U:O3'   | 39:DE:123:ALA:HB3  | 2.05                     | 0.57              |
| 40:DF:187:VAL:HG12 | 48:DP:7:ARG:NH2    | 2.19                     | 0.57              |
| 40:DF:18:ARG:HG2   | 40:DF:19:GLU:N     | 2.18                     | 0.57              |
| 41:DG:181:ARG:CZ   | 41:DG:181:ARG:HB2  | 2.33                     | 0.57              |
| 48:DP:23:PRO:C     | 48:DP:33:ARG:CZ    | 2.73                     | 0.57              |
| 57:DY:28:LYS:O     | 57:DY:38:ILE:HG22  | 2.04                     | 0.57              |
| 1:AA:1254:C:H2'    | 1:AA:1255:G:C8     | 2.40                     | 0.57              |
| 1:AA:1490:C:H5'    | 1:AA:1490:C:H6     | 1.69                     | 0.57              |
| 2:AB:96:ARG:N      | 2:AB:96:ARG:HD2    | 2.19                     | 0.57              |
| 3:AC:14:ILE:O      | 3:AC:15:THR:HB     | 2.04                     | 0.57              |
| 6:AF:36:ARG:NH1    | 6:AF:36:ARG:HB3    | 2.19                     | 0.57              |
| 11:AK:21:ILE:HG13  | 11:AK:30:VAL:HG12  | 1.87                     | 0.57              |
| 11:AK:79:SER:OG    | 11:AK:106:LYS:HD2  | 2.04                     | 0.57              |
| 13:AM:74:VAL:O     | 13:AM:77:ASN:HB2   | 2.03                     | 0.57              |
| 19:AS:21:GLU:HG3   | 19:AS:22:LEU:CD2   | 2.34                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:AY:630:GLN:HG2  | 24:AY:630:GLN:O   | 2.04                     | 0.57              |
| 31:B6:30:THR:HG22  | 31:B6:32:ASN:ND2  | 2.19                     | 0.57              |
| 35:BA:1353:A:H2'   | 35:BA:1354:A:C8   | 2.39                     | 0.57              |
| 35:BA:1473:G:H2'   | 35:BA:1474:C:O4'  | 2.04                     | 0.57              |
| 35:BA:1677:A:H2'   | 35:BA:1678:G:C8   | 2.40                     | 0.57              |
| 35:BA:1943:U:O2'   | 35:BA:1944:U:O5'  | 2.17                     | 0.57              |
| 35:BA:1949:G:H2'   | 35:BA:1950:G:C8   | 2.39                     | 0.57              |
| 35:BA:2097:C:H2'   | 35:BA:2098:U:C6   | 2.39                     | 0.57              |
| 33:B8:62:LEU:CD1   | 35:BA:242:G:H5''  | 2.33                     | 0.57              |
| 35:BA:2450:A:O2'   | 35:BA:2451:A:H5'  | 2.04                     | 0.57              |
| 35:BA:2504:U:H6    | 35:BA:2504:U:O5'  | 1.87                     | 0.57              |
| 35:BA:27:G:O2'     | 35:BA:28:A:H8     | 1.86                     | 0.57              |
| 35:BA:737:C:C2'    | 35:BA:738:G:H5'   | 2.35                     | 0.57              |
| 35:BA:958:U:H5'    | 49:BQ:14:ARG:HH11 | 1.69                     | 0.57              |
| 37:BC:117:THR:HG22 | 37:BC:147:GLY:O   | 2.04                     | 0.57              |
| 38:BD:142:VAL:HG23 | 38:BD:192:THR:C   | 2.25                     | 0.57              |
| 38:BD:65:ILE:N     | 38:BD:65:ILE:HD13 | 2.19                     | 0.57              |
| 29:B4:1:MET:HE2    | 41:BG:66:GLN:CD   | 2.25                     | 0.57              |
| 44:BK:8:VAL:HG12   | 44:BK:10:LEU:HG   | 1.86                     | 0.57              |
| 45:BL:79:UNK:C     | 45:BL:81:UNK:N    | 2.64                     | 0.57              |
| 46:BN:46:VAL:CG1   | 46:BN:47:ALA:H    | 2.13                     | 0.57              |
| 46:BN:4:TYR:CD1    | 46:BN:4:TYR:N     | 2.72                     | 0.57              |
| 46:BN:82:LEU:HD23  | 46:BN:82:LEU:C    | 2.24                     | 0.57              |
| 49:BQ:27:VAL:H     | 49:BQ:137:TYR:HD2 | 1.53                     | 0.57              |
| 52:BT:80:SER:CB    | 52:BT:81:PRO:CD   | 2.82                     | 0.57              |
| 53:BU:70:ARG:HA    | 53:BU:74:LEU:O    | 2.04                     | 0.57              |
| 1:CA:415:A:H2'     | 1:CA:416:G:C8     | 2.40                     | 0.57              |
| 1:CA:973:G:C1'     | 10:CJ:55:LYS:CE   | 2.82                     | 0.57              |
| 6:CF:69:GLU:H      | 6:CF:69:GLU:CD    | 2.07                     | 0.57              |
| 16:CP:50:LYS:O     | 16:CP:51:VAL:HG23 | 2.04                     | 0.57              |
| 24:CY:635:GLU:OE2  | 24:CY:644:ARG:NH1 | 2.38                     | 0.57              |
| 27:D2:38:GLN:HA    | 27:D2:41:ILE:CG2  | 2.34                     | 0.57              |
| 42:DH:159:GLU:HA   | 42:DH:159:GLU:OE1 | 2.04                     | 0.57              |
| 49:DQ:2:LEU:HG     | 49:DQ:69:PHE:HE1  | 1.70                     | 0.57              |
| 49:DQ:76:LYS:HB3   | 49:DQ:91:GLU:CG   | 2.34                     | 0.57              |
| 50:DR:44:LEU:HD13  | 50:DR:44:LEU:O    | 2.04                     | 0.57              |
| 51:DS:28:VAL:CG1   | 51:DS:29:PHE:H    | 2.12                     | 0.57              |
| 58:DZ:127:LYS:HE2  | 58:DZ:162:GLU:OE2 | 2.05                     | 0.57              |
| 1:AA:191:G:H1'     | 20:AT:105:SER:HA  | 1.86                     | 0.57              |
| 1:AA:370:C:O2'     | 1:AA:371:G:H5'    | 2.04                     | 0.57              |
| 13:AM:68:GLY:H     | 13:AM:71:ARG:CB   | 2.15                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 16:AP:74:LEU:O     | 16:AP:79:VAL:HG23 | 2.04                     | 0.57              |
| 19:AS:48:THR:HG22  | 19:AS:61:TYR:HA   | 1.86                     | 0.57              |
| 24:AY:137:ASN:HD21 | 24:AY:263:ALA:CB  | 2.18                     | 0.57              |
| 24:AY:409:ILE:HD11 | 24:AY:654:GLY:CA  | 2.27                     | 0.57              |
| 26:B1:86:SER:HB2   | 26:B1:90:ILE:CD1  | 2.35                     | 0.57              |
| 29:B4:22:ILE:HG22  | 29:B4:23:GLU:N    | 2.19                     | 0.57              |
| 35:BA:2647:U:H2'   | 35:BA:2648:C:C6   | 2.39                     | 0.57              |
| 38:BD:241:PRO:C    | 38:BD:242:ARG:HG3 | 2.24                     | 0.57              |
| 40:BF:8:GLN:NE2    | 40:BF:9:ILE:HB    | 2.20                     | 0.57              |
| 35:BA:1036:G:OP2   | 42:BH:59:ARG:NH1  | 2.38                     | 0.57              |
| 44:BK:24:GLY:H     | 44:BK:25:PRO:HD2  | 1.68                     | 0.57              |
| 48:BP:112:LEU:O    | 48:BP:128:HIS:HB2 | 2.04                     | 0.57              |
| 49:BQ:55:VAL:HG13  | 49:BQ:56:ARG:N    | 2.18                     | 0.57              |
| 51:BS:64:GLU:H     | 51:BS:64:GLU:CD   | 2.07                     | 0.57              |
| 52:BT:29:ARG:CG    | 52:BT:85:LYS:HA   | 2.33                     | 0.57              |
| 35:BA:1322:A:OP1   | 55:BW:11:ARG:HG3  | 2.04                     | 0.57              |
| 55:BW:36:LEU:HD11  | 55:BW:47:VAL:HG12 | 1.86                     | 0.57              |
| 1:CA:1237:C:OP1    | 1:CA:1238:A:H1'   | 2.05                     | 0.57              |
| 1:CA:957:U:H2'     | 1:CA:959:A:OP2    | 2.04                     | 0.57              |
| 2:CB:11:LEU:HD11   | 2:CB:217:ARG:NH2  | 2.19                     | 0.57              |
| 5:CE:15:ARG:HG3    | 5:CE:28:PHE:CE2   | 2.39                     | 0.57              |
| 11:CK:79:SER:OG    | 11:CK:106:LYS:HD2 | 2.04                     | 0.57              |
| 17:CQ:48:GLU:O     | 17:CQ:50:LYS:N    | 2.37                     | 0.57              |
| 19:CS:78:ARG:HB2   | 19:CS:81:ARG:NH1  | 2.17                     | 0.57              |
| 24:CY:112:GLN:HG3  | 24:CY:115:GLU:HB3 | 1.85                     | 0.57              |
| 24:CY:589:ALA:O    | 24:CY:593:ALA:HB2 | 2.03                     | 0.57              |
| 31:D6:18:ARG:HG3   | 31:D6:19:ARG:H    | 1.69                     | 0.57              |
| 32:D7:24:THR:HG23  | 32:D7:27:GLY:HA3  | 1.87                     | 0.57              |
| 35:DA:1248:G:C2    | 53:DU:3:ARG:HD2   | 2.38                     | 0.57              |
| 35:DA:1274:A:N3    | 35:DA:1297:C:H1'  | 2.19                     | 0.57              |
| 35:DA:1374:G:H2'   | 35:DA:1375:C:C6   | 2.40                     | 0.57              |
| 35:DA:1386:C:H2'   | 35:DA:1387:C:C6   | 2.40                     | 0.57              |
| 35:DA:2453:A:H2'   | 35:DA:2454:G:H8   | 1.69                     | 0.57              |
| 35:DA:2504:U:H6    | 35:DA:2504:U:O5'  | 1.88                     | 0.57              |
| 35:DA:803:U:H2'    | 35:DA:804:A:H5'   | 1.86                     | 0.57              |
| 38:DD:9:TYR:C      | 38:DD:10:THR:HG22 | 2.24                     | 0.57              |
| 39:DE:34:VAL:O     | 39:DE:35:GLN:CB   | 2.53                     | 0.57              |
| 40:DF:2:LYS:HG3    | 40:DF:25:PRO:HG2  | 1.86                     | 0.57              |
| 40:DF:75:HIS:HE1   | 40:DF:82:ILE:HD11 | 1.69                     | 0.57              |
| 41:DG:61:ALA:HA    | 41:DG:64:THR:CG2  | 2.35                     | 0.57              |
| 48:DP:124:LYS:CD   | 48:DP:143:GLY:HA3 | 2.35                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 48:DP:66:GLY:O     | 48:DP:67:MET:HB3  | 2.04                     | 0.57              |
| 51:DS:42:ASP:C     | 51:DS:44:LYS:H    | 2.08                     | 0.57              |
| 2:AB:155:LEU:HD13  | 2:AB:155:LEU:C    | 2.24                     | 0.57              |
| 3:AC:119:ARG:O     | 3:AC:123:GLN:HG3  | 2.03                     | 0.57              |
| 15:AO:74:ASP:C     | 15:AO:76:GLU:H    | 2.06                     | 0.57              |
| 20:AT:26:ASN:O     | 20:AT:30:LYS:HB2  | 2.04                     | 0.57              |
| 22:AV:71:C:O2      | 22:AV:71:C:C2'    | 2.53                     | 0.57              |
| 23:AX:19:U:H2'     | 23:AX:20:U:C6     | 2.40                     | 0.57              |
| 24:AY:13:ARG:HB2   | 24:AY:79:ILE:HG12 | 1.87                     | 0.57              |
| 28:B3:11:SER:HB3   | 35:BA:988:A:P     | 2.45                     | 0.57              |
| 31:B6:27:LYS:HB3   | 31:B6:30:THR:HG22 | 1.87                     | 0.57              |
| 35:BA:1301:A:H4'   | 35:BA:1302:A:OP1  | 2.04                     | 0.57              |
| 35:BA:1301:A:O2'   | 35:BA:1302:A:C2'  | 2.46                     | 0.57              |
| 35:BA:145:G:H2'    | 35:BA:146:G:C8    | 2.39                     | 0.57              |
| 35:BA:271(I):G:H3' | 35:BA:271(J):C:H6 | 1.68                     | 0.57              |
| 38:BD:80:ALA:HB3   | 38:BD:94:LEU:HB3  | 1.87                     | 0.57              |
| 40:BF:125:LEU:HD23 | 40:BF:125:LEU:N   | 2.18                     | 0.57              |
| 41:BG:133:LEU:HD12 | 41:BG:157:ILE:HB  | 1.87                     | 0.57              |
| 44:BK:112:MET:N    | 44:BK:113:PRO:HD2 | 2.20                     | 0.57              |
| 46:BN:17:ASP:CG    | 46:BN:56:ASN:HB3  | 2.25                     | 0.57              |
| 48:BP:105:LEU:HD12 | 48:BP:105:LEU:N   | 2.18                     | 0.57              |
| 49:BQ:27:VAL:O     | 49:BQ:28:ALA:HB3  | 2.04                     | 0.57              |
| 49:BQ:97:VAL:HG21  | 49:BQ:103:MET:HE3 | 1.85                     | 0.57              |
| 50:BR:83:ILE:O     | 50:BR:87:TYR:HE2  | 1.87                     | 0.57              |
| 51:BS:106:ARG:HD2  | 51:BS:106:ARG:C   | 2.24                     | 0.57              |
| 51:BS:54:LEU:HD13  | 51:BS:54:LEU:O    | 2.04                     | 0.57              |
| 51:BS:59:LYS:CD    | 51:BS:61:ASN:HB2  | 2.34                     | 0.57              |
| 51:BS:98:VAL:CG1   | 51:BS:100:ALA:HB2 | 2.35                     | 0.57              |
| 54:BV:18:LEU:CD1   | 54:BV:19:LYS:H    | 2.17                     | 0.57              |
| 57:BY:2:ARG:CD     | 57:BY:3:VAL:HG23  | 2.34                     | 0.57              |
| 57:BY:8:LYS:HD2    | 57:BY:8:LYS:H     | 1.68                     | 0.57              |
| 1:CA:1325:C:H2'    | 1:CA:1326:C:C6    | 2.40                     | 0.57              |
| 1:CA:260:G:H2'     | 1:CA:261:U:H6     | 1.70                     | 0.57              |
| 4:CD:114:ARG:HG3   | 4:CD:114:ARG:NH1  | 2.17                     | 0.57              |
| 9:CI:41:VAL:HG12   | 9:CI:41:VAL:O     | 2.05                     | 0.57              |
| 19:CS:29:ARG:O     | 19:CS:31:ILE:HG22 | 2.04                     | 0.57              |
| 26:D1:93:GLU:O     | 26:D1:95:LEU:N    | 2.36                     | 0.57              |
| 33:D8:62:LEU:CD1   | 35:DA:242:G:H5''  | 2.32                     | 0.57              |
| 35:DA:139(A):G:N2  | 56:DX:44:GLU:OE1  | 2.38                     | 0.57              |
| 35:DA:2111:C:C2    | 35:DA:2147:G:N2   | 2.73                     | 0.57              |
| 35:DA:2230:G:H2'   | 35:DA:2231:C:H6   | 1.70                     | 0.57              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:35:G:O2'     | 35:DA:36:G:H5'     | 2.04                     | 0.57              |
| 35:DA:962:G:H2'    | 35:DA:963:U:O4'    | 2.05                     | 0.57              |
| 39:DE:111:ARG:HA   | 50:DR:2:ARG:CB     | 2.31                     | 0.57              |
| 44:DK:109:LYS:HA   | 44:DK:112:MET:HE2  | 1.85                     | 0.57              |
| 46:DN:82:LEU:HD23  | 46:DN:82:LEU:C     | 2.25                     | 0.57              |
| 49:DQ:62:GLY:O     | 58:DZ:178:GLU:HB2  | 2.03                     | 0.57              |
| 52:DT:55:ASN:N     | 52:DT:59:THR:CG2   | 2.63                     | 0.57              |
| 57:DY:2:ARG:CD     | 57:DY:3:VAL:HG23   | 2.35                     | 0.57              |
| 58:DZ:127:LYS:HZ3  | 58:DZ:127:LYS:HB3  | 1.68                     | 0.57              |
| 1:AA:474:G:H2'     | 1:AA:475:G:C8      | 2.40                     | 0.57              |
| 11:AK:21:ILE:N     | 11:AK:21:ILE:HD12  | 2.20                     | 0.57              |
| 24:AY:171:GLU:HG3  | 24:AY:172:ASP:H    | 1.70                     | 0.57              |
| 24:AY:604:PRO:HB2  | 24:AY:649:LEU:HD12 | 1.87                     | 0.57              |
| 26:B1:80:LEU:HD23  | 26:B1:81:LYS:N     | 2.13                     | 0.57              |
| 29:B4:1:MET:HG3    | 41:BG:66:GLN:HG3   | 1.87                     | 0.57              |
| 30:B5:3:LYS:HZ1    | 35:BA:2613:U:C2'   | 2.18                     | 0.57              |
| 31:B6:45:LYS:HG2   | 35:BA:2371:G:H5''  | 1.86                     | 0.57              |
| 31:B6:15:GLU:CB    | 31:B6:47:THR:HG21  | 2.34                     | 0.57              |
| 33:B8:14:VAL:HG21  | 33:B8:22:VAL:CG1   | 2.35                     | 0.57              |
| 35:BA:1614:A:H2'   | 35:BA:1615:C:H5'   | 1.86                     | 0.57              |
| 35:BA:2307:G:C2    | 35:BA:2308:G:H5''  | 2.38                     | 0.57              |
| 35:BA:877:U:O2'    | 35:BA:878:A:H5''   | 2.05                     | 0.57              |
| 35:BA:881:G:H2'    | 35:BA:882:G:H5'    | 1.86                     | 0.57              |
| 38:BD:146:GLU:HB2  | 38:BD:189:CYS:HB3  | 1.87                     | 0.57              |
| 40:BF:185:ASP:HA   | 40:BF:188:ARG:HG2  | 1.85                     | 0.57              |
| 42:BH:89:ILE:O     | 42:BH:89:ILE:HG13  | 2.05                     | 0.57              |
| 48:BP:91:PHE:CE2   | 48:BP:95:VAL:HG12  | 2.40                     | 0.57              |
| 52:BT:51:ARG:O     | 52:BT:61:PHE:HA    | 2.03                     | 0.57              |
| 53:BU:33:ARG:C     | 53:BU:35:ALA:N     | 2.56                     | 0.57              |
| 56:BX:12:VAL:O     | 56:BX:13:LEU:HB2   | 2.05                     | 0.57              |
| 57:BY:73:ARG:O     | 57:BY:74:PRO:O     | 2.23                     | 0.57              |
| 58:BZ:141:VAL:O    | 58:BZ:142:SER:HB3  | 2.03                     | 0.57              |
| 58:BZ:154:ASP:N    | 58:BZ:154:ASP:OD2  | 2.35                     | 0.57              |
| 3:CC:52:LEU:HD23   | 3:CC:52:LEU:N      | 2.14                     | 0.57              |
| 4:CD:11:LEU:O      | 4:CD:12:CYS:C      | 2.42                     | 0.57              |
| 4:CD:203:VAL:O     | 4:CD:206:PHE:HB3   | 2.05                     | 0.57              |
| 4:CD:8:VAL:HB      | 4:CD:21:LEU:CD1    | 2.34                     | 0.57              |
| 13:CM:81:LEU:HD22  | 13:CM:81:LEU:N     | 2.20                     | 0.57              |
| 24:CY:146:LEU:HD11 | 24:CY:260:LEU:HD11 | 1.87                     | 0.57              |
| 26:D1:23:LYS:CE    | 26:D1:28:GLY:HA3   | 2.26                     | 0.57              |
| 29:D4:22:ILE:HG22  | 29:D4:23:GLU:N     | 2.20                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 33:D8:7:HIS:HB3    | 33:D8:10:ALA:HB3  | 1.87                     | 0.57              |
| 35:DA:1169:G:H1    | 35:DA:1180:C:H42  | 1.50                     | 0.57              |
| 35:DA:2317:C:H2'   | 35:DA:2318:G:C5'  | 2.31                     | 0.57              |
| 35:DA:2464:C:HO2'  | 35:DA:2465:C:H6   | 1.52                     | 0.57              |
| 35:DA:363(B):G:H2' | 35:DA:363(C):G:C8 | 2.38                     | 0.57              |
| 35:DA:610:G:N2     | 35:DA:619:G:H1'   | 2.20                     | 0.57              |
| 35:DA:621:A:H2'    | 35:DA:622:G:C5'   | 2.33                     | 0.57              |
| 35:DA:259:G:H21    | 35:DA:621:A:H8    | 1.51                     | 0.57              |
| 39:DE:69:LYS:N     | 39:DE:69:LYS:HE2  | 2.19                     | 0.57              |
| 42:DH:83:TYR:O     | 42:DH:84:SER:HB3  | 2.05                     | 0.57              |
| 44:DK:3:LYS:HB3    | 44:DK:29:GLN:HB3  | 1.85                     | 0.57              |
| 48:DP:105:LEU:HD12 | 48:DP:105:LEU:N   | 2.19                     | 0.57              |
| 48:DP:84:ASN:C     | 48:DP:86:LYS:N    | 2.58                     | 0.57              |
| 49:DQ:27:VAL:H     | 49:DQ:137:TYR:HD2 | 1.53                     | 0.57              |
| 52:DT:53:ARG:HH11  | 52:DT:53:ARG:CB   | 2.17                     | 0.57              |
| 35:DA:328:U:H4'    | 57:DY:68:HIS:CD2  | 2.39                     | 0.57              |
| 57:DY:96:ILE:CG2   | 57:DY:99:CYS:HB3  | 2.34                     | 0.57              |
| 1:AA:1015:A:H2'    | 1:AA:1016:A:C8    | 2.40                     | 0.57              |
| 1:AA:1226:C:H4'    | 1:AA:1227:A:OP1   | 2.05                     | 0.57              |
| 1:AA:1404:C:H1'    | 1:AA:1499:A:N1    | 2.19                     | 0.57              |
| 1:AA:954:G:H2'     | 1:AA:955:U:C6     | 2.40                     | 0.57              |
| 1:AA:542:G:H5'     | 4:AD:41:GLY:CA    | 2.35                     | 0.57              |
| 5:AE:36:ASP:OD1    | 5:AE:38:GLN:N     | 2.26                     | 0.57              |
| 24:AY:210:ARG:O    | 24:AY:213:HIS:N   | 2.34                     | 0.57              |
| 24:AY:463:VAL:O    | 24:AY:467:LYS:HB3 | 2.05                     | 0.57              |
| 27:B2:14:ARG:HH11  | 27:B2:14:ARG:HG3  | 1.69                     | 0.57              |
| 30:B5:44:THR:O     | 30:B5:51:TYR:HE1  | 1.87                     | 0.57              |
| 34:B9:34:GLN:O     | 34:B9:35:ARG:HB2  | 2.03                     | 0.57              |
| 35:BA:1198:U:H2'   | 35:BA:1198:U:O2   | 2.03                     | 0.57              |
| 35:BA:1669:A:H2'   | 35:BA:1670:C:H5'  | 1.86                     | 0.57              |
| 35:BA:200:U:H2'    | 35:BA:201:C:H5'   | 1.86                     | 0.57              |
| 35:BA:608:A:H2'    | 35:BA:609:A:C8    | 2.39                     | 0.57              |
| 35:BA:610:G:N2     | 35:BA:619:G:H1'   | 2.19                     | 0.57              |
| 35:BA:764:A:N3     | 38:BD:213:ARG:NH1 | 2.53                     | 0.57              |
| 36:BB:7:G:C3'      | 36:BB:8:U:H5'     | 2.34                     | 0.57              |
| 37:BC:185:LYS:HE3  | 37:BC:185:LYS:HA  | 1.87                     | 0.57              |
| 42:BH:45:VAL:HA    | 42:BH:50:VAL:HG22 | 1.87                     | 0.57              |
| 46:BN:62:VAL:HG13  | 46:BN:62:VAL:O    | 2.05                     | 0.57              |
| 48:BP:23:PRO:CB    | 48:BP:33:ARG:HG3  | 2.33                     | 0.57              |
| 49:BQ:44:ALA:N     | 49:BQ:45:GLN:HE21 | 2.02                     | 0.57              |
| 51:BS:42:ASP:C     | 51:BS:44:LYS:H    | 2.07                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:BZ:23:LYS:CD    | 58:BZ:38:TYR:HE1   | 2.12                     | 0.57              |
| 1:CA:1324:A:H2'    | 1:CA:1325:C:H6     | 1.68                     | 0.57              |
| 1:CA:291:C:O2'     | 1:CA:292:G:H5'     | 2.04                     | 0.57              |
| 1:CA:624:C:H2'     | 1:CA:625:G:H8      | 1.69                     | 0.57              |
| 2:CB:51:LEU:HD21   | 2:CB:201:ILE:HG23  | 1.87                     | 0.57              |
| 4:CD:162:LEU:HD11  | 4:CD:181:MET:CG    | 2.34                     | 0.57              |
| 8:CH:7:ALA:HB2     | 8:CH:85:ARG:HD3    | 1.86                     | 0.57              |
| 10:CJ:32:ALA:N     | 10:CJ:78:ASN:ND2   | 2.53                     | 0.57              |
| 17:CQ:7:THR:O      | 17:CQ:23:VAL:HG13  | 2.04                     | 0.57              |
| 24:CY:487:ILE:H    | 24:CY:487:ILE:HD13 | 1.68                     | 0.57              |
| 35:DA:207:A:H2'    | 35:DA:208:C:O4'    | 2.03                     | 0.57              |
| 35:DA:226:G:O2'    | 35:DA:227:A:C8     | 2.45                     | 0.57              |
| 35:DA:285:C:H2'    | 35:DA:286:C:H5'    | 1.86                     | 0.57              |
| 37:DC:215:VAL:HG23 | 37:DC:225:ILE:HG12 | 1.86                     | 0.57              |
| 37:DC:92:ALA:HB2   | 37:DC:154:ILE:HD13 | 1.85                     | 0.57              |
| 35:DA:1774:C:O2    | 38:DD:11:PRO:HB2   | 2.04                     | 0.57              |
| 40:DF:167:ALA:CB   | 40:DF:173:VAL:HG11 | 2.23                     | 0.57              |
| 46:DN:4:TYR:CD1    | 46:DN:4:TYR:N      | 2.72                     | 0.57              |
| 49:DQ:27:VAL:HG21  | 49:DQ:134:ARG:HG2  | 1.87                     | 0.57              |
| 49:DQ:27:VAL:O     | 49:DQ:28:ALA:HB3   | 2.04                     | 0.57              |
| 49:DQ:53:ALA:HA    | 49:DQ:56:ARG:HB2   | 1.86                     | 0.57              |
| 50:DR:21:TYR:HB3   | 50:DR:47:PHE:CE2   | 2.39                     | 0.57              |
| 51:DS:20:ARG:HA    | 51:DS:20:ARG:NE    | 2.19                     | 0.57              |
| 52:DT:10:VAL:C     | 52:DT:12:SER:N     | 2.58                     | 0.57              |
| 52:DT:42:ILE:HD13  | 52:DT:83:ILE:HD13  | 1.87                     | 0.57              |
| 54:DV:51:VAL:HG12  | 54:DV:52:VAL:N     | 2.14                     | 0.57              |
| 1:AA:67:C:H2'      | 1:AA:68:G:C8       | 2.40                     | 0.57              |
| 6:AF:9:VAL:HB      | 6:AF:87:ARG:HB2    | 1.85                     | 0.57              |
| 1:AA:689:C:P       | 11:AK:46:GLY:HA3   | 2.45                     | 0.57              |
| 19:AS:53:ASN:O     | 19:AS:55:LYS:N     | 2.38                     | 0.57              |
| 19:AS:6:LYS:H      | 19:AS:6:LYS:HE3    | 1.69                     | 0.57              |
| 19:AS:9:VAL:HG23   | 29:B4:53:GLU:OE2   | 2.04                     | 0.57              |
| 22:AW:28:U:H2'     | 22:AW:29:C:H6      | 1.69                     | 0.57              |
| 24:AY:273:LEU:HA   | 24:AY:276:VAL:HG23 | 1.85                     | 0.57              |
| 24:AY:343:ASN:ND2  | 24:AY:345:THR:N    | 2.52                     | 0.57              |
| 29:B4:37:SER:O     | 29:B4:38:LYS:HB2   | 2.05                     | 0.57              |
| 35:BA:1416:G:HO2'  | 35:BA:1417:C:H5    | 1.52                     | 0.57              |
| 35:BA:1516:C:O2'   | 35:BA:1517:G:H5''  | 2.04                     | 0.57              |
| 35:BA:2008:C:H2'   | 35:BA:2009:G:C8    | 2.39                     | 0.57              |
| 35:BA:226:G:O2'    | 35:BA:227:A:C8     | 2.47                     | 0.57              |
| 35:BA:2850:A:H5'   | 35:BA:2868:A:H2    | 1.70                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:BA:947:G:H2'   | 35:BA:948:G:C8     | 2.40                     | 0.57              |
| 39:BE:69:LYS:N    | 39:BE:69:LYS:HE2   | 2.20                     | 0.57              |
| 41:BG:101:ILE:O   | 41:BG:104:GLU:HB3  | 2.05                     | 0.57              |
| 41:BG:113:ARG:O   | 41:BG:140:ILE:HG22 | 2.04                     | 0.57              |
| 46:BN:7:LYS:O     | 46:BN:9:VAL:N      | 2.37                     | 0.57              |
| 48:BP:124:LYS:CD  | 48:BP:143:GLY:HA3  | 2.35                     | 0.57              |
| 49:BQ:12:GLN:NE2  | 49:BQ:73:PRO:HD2   | 2.20                     | 0.57              |
| 52:BT:132:LYS:HG2 | 52:BT:133:GLU:N    | 2.20                     | 0.57              |
| 54:BV:2:PHE:CE1   | 54:BV:13:ARG:NH1   | 2.73                     | 0.57              |
| 57:BY:12:THR:HG22 | 57:BY:75:ILE:HG21  | 1.87                     | 0.57              |
| 57:BY:76:CYS:HB3  | 57:BY:96:ILE:CD1   | 2.24                     | 0.57              |
| 7:CG:146:GLU:HA   | 7:CG:149:ARG:HB2   | 1.86                     | 0.57              |
| 8:CH:9:MET:O      | 8:CH:13:ILE:HG12   | 2.04                     | 0.57              |
| 13:CM:33:ALA:HA   | 13:CM:59:TYR:HE2   | 1.70                     | 0.57              |
| 18:CR:74:ARG:HD3  | 18:CR:81:PHE:HD2   | 1.70                     | 0.57              |
| 24:CY:616:TYR:HB2 | 24:CY:663:THR:HG22 | 1.87                     | 0.57              |
| 24:CY:630:GLN:NE2 | 24:CY:646:PHE:CD2  | 2.72                     | 0.57              |
| 24:CY:680:PRO:O   | 24:CY:682:GLN:N    | 2.36                     | 0.57              |
| 26:D1:4:VAL:HG23  | 26:D1:10:LYS:O     | 2.04                     | 0.57              |
| 27:D2:59:ARG:O    | 27:D2:62:THR:N     | 2.38                     | 0.57              |
| 31:D6:15:GLU:CD   | 31:D6:44:ARG:HH12  | 2.08                     | 0.57              |
| 31:D6:37:ARG:O    | 31:D6:48:VAL:O     | 2.23                     | 0.57              |
| 33:D8:32:LEU:HB3  | 33:D8:36:LYS:NZ    | 2.20                     | 0.57              |
| 27:D2:69:ARG:NH2  | 35:DA:111:A:H5'    | 2.12                     | 0.57              |
| 35:DA:2850:A:H5'  | 35:DA:2868:A:H2    | 1.69                     | 0.57              |
| 35:DA:455:C:N3    | 35:DA:472:A:H2'    | 2.20                     | 0.57              |
| 35:DA:621:A:C2'   | 35:DA:622:G:H5'    | 2.35                     | 0.57              |
| 35:DA:6:A:N3      | 35:DA:6:A:H2'      | 2.18                     | 0.57              |
| 37:DC:139:PRO:HA  | 37:DC:145:THR:CG2  | 2.35                     | 0.57              |
| 38:DD:72:LYS:HB3  | 38:DD:75:ILE:HB    | 1.86                     | 0.57              |
| 35:DA:674:G:C1'   | 40:DF:74:ARG:HD3   | 2.33                     | 0.57              |
| 35:DA:1258:C:O4'  | 40:DF:84:VAL:HG21  | 2.05                     | 0.57              |
| 43:DJ:10:UNK:O    | 43:DJ:11:UNK:CB    | 2.53                     | 0.57              |
| 47:DO:60:ALA:HA   | 47:DO:87:ILE:HD13  | 1.86                     | 0.57              |
| 49:DQ:44:ALA:N    | 49:DQ:45:GLN:HE21  | 2.02                     | 0.57              |
| 50:DR:18:LEU:HD23 | 50:DR:18:LEU:C     | 2.24                     | 0.57              |
| 58:DZ:110:GLY:O   | 58:DZ:114:GLY:O    | 2.22                     | 0.57              |
| 1:AA:1478:C:O2'   | 1:AA:1479:C:H5'    | 2.04                     | 0.57              |
| 1:AA:630:G:C2'    | 1:AA:631:G:C5'     | 2.82                     | 0.57              |
| 1:AA:687:A:H62    | 1:AA:703:G:H1'     | 1.69                     | 0.57              |
| 5:AE:12:LEU:CD1   | 5:AE:31:LEU:HB3    | 2.35                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:AM:63:THR:HG22  | 13:AM:64:TRP:H     | 1.67                     | 0.57              |
| 19:AS:64:GLU:O     | 29:B4:48:ARG:NH2   | 2.37                     | 0.57              |
| 20:AT:47:GLY:O     | 20:AT:49:ALA:N     | 2.32                     | 0.57              |
| 24:AY:141:LYS:O    | 24:AY:144:ALA:HB2  | 2.05                     | 0.57              |
| 24:AY:209:ALA:O    | 24:AY:210:ARG:C    | 2.43                     | 0.57              |
| 24:AY:379:GLY:O    | 24:AY:380:LEU:HB2  | 2.04                     | 0.57              |
| 24:AY:395:PRO:O    | 24:AY:397:VAL:HG13 | 2.05                     | 0.57              |
| 24:AY:99:ARG:NE    | 24:AY:128:TYR:HB2  | 2.20                     | 0.57              |
| 30:B5:3:LYS:NZ     | 35:BA:2613:U:H2'   | 2.20                     | 0.57              |
| 35:BA:1809:A:H2'   | 35:BA:1810:A:C8    | 2.40                     | 0.57              |
| 35:BA:622:G:O2'    | 35:BA:623:G:H5'    | 2.05                     | 0.57              |
| 35:BA:889:C:H2'    | 35:BA:890:A:O4'    | 2.04                     | 0.57              |
| 38:BD:26:LYS:O     | 38:BD:27:THR:HG22  | 2.05                     | 0.57              |
| 38:BD:76:PRO:O     | 38:BD:98:VAL:HG23  | 2.03                     | 0.57              |
| 39:BE:34:VAL:O     | 39:BE:35:GLN:CB    | 2.52                     | 0.57              |
| 48:BP:12:ALA:HB1   | 48:BP:16:ARG:HB3   | 1.87                     | 0.57              |
| 49:BQ:76:LYS:HB3   | 49:BQ:91:GLU:CG    | 2.35                     | 0.57              |
| 35:BA:1248:G:C2    | 53:BU:3:ARG:HD2    | 2.40                     | 0.57              |
| 53:BU:65:ILE:HG12  | 53:BU:96:ALA:HB1   | 1.87                     | 0.57              |
| 57:BY:74:PRO:HG3   | 57:BY:83:THR:HG22  | 1.85                     | 0.57              |
| 58:BZ:107:THR:HG23 | 58:BZ:111:VAL:CB   | 2.35                     | 0.57              |
| 1:CA:1416:G:H2'    | 1:CA:1417:G:O4'    | 2.05                     | 0.57              |
| 2:CB:101:MET:C     | 2:CB:102:LEU:HD12  | 2.25                     | 0.57              |
| 2:CB:223:ILE:C     | 2:CB:225:ALA:H     | 2.08                     | 0.57              |
| 5:CE:79:GLU:HB3    | 5:CE:93:PRO:HD2    | 1.87                     | 0.57              |
| 6:CF:67:MET:SD     | 6:CF:75:LEU:HD22   | 2.44                     | 0.57              |
| 7:CG:113:GLU:HG2   | 7:CG:119:ARG:HG2   | 1.87                     | 0.57              |
| 7:CG:38:LEU:O      | 7:CG:41:ARG:HB2    | 2.05                     | 0.57              |
| 8:CH:104:ARG:O     | 8:CH:106:GLY:N     | 2.38                     | 0.57              |
| 24:CY:330:VAL:HG12 | 24:CY:331:TYR:H    | 1.70                     | 0.57              |
| 25:D0:45:PHE:O     | 25:D0:59:LEU:HD11  | 2.05                     | 0.57              |
| 35:DA:1301:A:HO2'  | 35:DA:1302:A:H2'   | 1.69                     | 0.57              |
| 35:DA:203:C:C3'    | 35:DA:204:A:H5''   | 2.30                     | 0.57              |
| 35:DA:2199:A:H3'   | 35:DA:2200:C:H6    | 1.68                     | 0.57              |
| 35:DA:2769:C:O2'   | 35:DA:2770:G:H5'   | 2.05                     | 0.57              |
| 37:DC:185:LYS:HE3  | 37:DC:185:LYS:HA   | 1.86                     | 0.57              |
| 44:DK:21:PRO:HA    | 44:DK:23:VAL:N     | 2.19                     | 0.57              |
| 46:DN:17:ASP:CG    | 46:DN:56:ASN:HB3   | 2.26                     | 0.57              |
| 35:DA:1141:U:H5''  | 46:DN:63:THR:HG23  | 1.85                     | 0.57              |
| 55:DW:36:LEU:HD11  | 55:DW:47:VAL:HG12  | 1.87                     | 0.57              |
| 57:DY:39:VAL:HG12  | 57:DY:40:GLU:N     | 2.20                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:DZ:10:ARG:NH2   | 58:DZ:26:GLY:O     | 2.38                     | 0.57              |
| 58:DZ:127:LYS:CB   | 58:DZ:127:LYS:NZ   | 2.68                     | 0.57              |
| 1:AA:1108:G:H5'    | 3:AC:176:HIS:CD2   | 2.40                     | 0.56              |
| 1:AA:1057:G:N2     | 1:AA:1204:A:H1'    | 2.20                     | 0.56              |
| 4:AD:17:VAL:O      | 4:AD:17:VAL:HG12   | 2.05                     | 0.56              |
| 10:AJ:33:GLN:N     | 10:AJ:75:ILE:HD11  | 2.20                     | 0.56              |
| 1:AA:449:C:O2      | 16:AP:42:ARG:HD2   | 2.05                     | 0.56              |
| 18:AR:44:LEU:CD2   | 18:AR:79:LEU:HD22  | 2.35                     | 0.56              |
| 24:AY:495:GLY:O    | 24:AY:509:HIS:HA   | 2.05                     | 0.56              |
| 27:B2:25:VAL:O     | 27:B2:27:GLU:N     | 2.37                     | 0.56              |
| 35:BA:1093:G:H21   | 35:BA:1098:A:H62   | 1.53                     | 0.56              |
| 35:BA:1109:C:H5'   | 35:BA:1110:G:OP2   | 2.04                     | 0.56              |
| 35:BA:1374:G:H2'   | 35:BA:1375:C:C6    | 2.39                     | 0.56              |
| 35:BA:1847:A:H3'   | 35:BA:1848:A:C5'   | 2.35                     | 0.56              |
| 35:BA:2305:A:H5''  | 41:BG:134:GLY:HA3  | 1.87                     | 0.56              |
| 35:BA:2556:C:H2'   | 35:BA:2557:G:O4'   | 2.05                     | 0.56              |
| 35:BA:2754:U:H2'   | 35:BA:2755:C:H5'   | 1.87                     | 0.56              |
| 35:BA:910:A:H62    | 49:BQ:12:GLN:HA    | 1.68                     | 0.56              |
| 35:BA:945:A:O2'    | 35:BA:946:G:H4'    | 2.05                     | 0.56              |
| 38:BD:23:GLU:HA    | 38:BD:23:GLU:OE1   | 2.04                     | 0.56              |
| 38:BD:71:ASP:HB2   | 38:BD:103:ARG:NH2  | 2.05                     | 0.56              |
| 39:BE:47:VAL:CG1   | 39:BE:48:GLN:H     | 2.13                     | 0.56              |
| 40:BF:152:GLU:O    | 40:BF:153:SER:C    | 2.43                     | 0.56              |
| 41:BG:91:ARG:C     | 41:BG:91:ARG:CD    | 2.73                     | 0.56              |
| 43:BJ:56:UNK:CB    | 43:BJ:83:UNK:HA    | 2.34                     | 0.56              |
| 44:BK:77:LEU:H     | 44:BK:77:LEU:CD2   | 2.09                     | 0.56              |
| 47:BO:97:ARG:HH11  | 47:BO:97:ARG:HG3   | 1.70                     | 0.56              |
| 48:BP:115:LEU:HD23 | 48:BP:115:LEU:H    | 1.70                     | 0.56              |
| 48:BP:146:VAL:O    | 48:BP:148:LEU:HD12 | 2.05                     | 0.56              |
| 52:BT:126:ALA:C    | 52:BT:128:GLU:H    | 2.08                     | 0.56              |
| 55:BW:25:ARG:NH2   | 55:BW:74:ALA:O     | 2.38                     | 0.56              |
| 57:BY:88:LYS:HD2   | 57:BY:88:LYS:N     | 2.19                     | 0.56              |
| 1:CA:833:U:H2'     | 1:CA:834:C:C6      | 2.40                     | 0.56              |
| 10:CJ:90:LEU:N     | 10:CJ:91:PRO:CD    | 2.68                     | 0.56              |
| 13:CM:121:LYS:HD3  | 13:CM:121:LYS:N    | 2.20                     | 0.56              |
| 25:D0:51:VAL:CG2   | 25:D0:81:VAL:HG23  | 2.34                     | 0.56              |
| 28:D3:4:LEU:O      | 28:D3:36:VAL:HA    | 2.04                     | 0.56              |
| 29:D4:37:SER:O     | 29:D4:38:LYS:HB2   | 2.04                     | 0.56              |
| 33:D8:25:MET:O     | 33:D8:47:LYS:HG2   | 2.05                     | 0.56              |
| 35:DA:1043:C:C3'   | 35:DA:1044:G:H5''  | 2.34                     | 0.56              |
| 35:DA:120:U:H5'    | 35:DA:121:G:OP1    | 2.04                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:1301:A:H4'   | 35:DA:1302:A:OP1   | 2.04                     | 0.56              |
| 35:DA:1485:G:C1'   | 35:DA:1505:C:H42   | 2.17                     | 0.56              |
| 35:DA:1718:G:H5'   | 35:DA:1718:G:C8    | 2.40                     | 0.56              |
| 35:DA:784:A:H5''   | 38:DD:227:ASN:HD21 | 1.70                     | 0.56              |
| 37:DC:118:PRO:HB2  | 37:DC:148:PHE:CZ   | 2.41                     | 0.56              |
| 38:DD:210:GLY:O    | 38:DD:212:SER:N    | 2.36                     | 0.56              |
| 38:DD:79:VAL:O     | 38:DD:113:VAL:HG13 | 2.04                     | 0.56              |
| 35:DA:2657:A:O2'   | 42:DH:160:LYS:HE3  | 2.05                     | 0.56              |
| 42:DH:89:ILE:O     | 42:DH:89:ILE:HG13  | 2.05                     | 0.56              |
| 51:DS:88:ASP:CG    | 51:DS:89:ARG:H     | 2.07                     | 0.56              |
| 53:DU:76:TYR:C     | 53:DU:76:TYR:CD2   | 2.78                     | 0.56              |
| 1:AA:950:U:H2'     | 1:AA:951:G:H8      | 1.70                     | 0.56              |
| 7:AG:153:HIS:CE1   | 11:AK:58:PRO:HD2   | 2.41                     | 0.56              |
| 12:AL:25:PRO:C     | 12:AL:27:LEU:N     | 2.54                     | 0.56              |
| 17:AQ:7:THR:O      | 17:AQ:23:VAL:HG13  | 2.04                     | 0.56              |
| 19:AS:29:ARG:O     | 19:AS:31:ILE:HG22  | 2.05                     | 0.56              |
| 20:AT:24:LEU:O     | 20:AT:24:LEU:HD13  | 2.05                     | 0.56              |
| 24:AY:113:GLY:C    | 24:AY:115:GLU:N    | 2.48                     | 0.56              |
| 24:AY:534:ILE:HG13 | 24:AY:570:GLY:O    | 2.05                     | 0.56              |
| 24:AY:435:ASP:OD1  | 61:AY:702:FUA:H22  | 2.05                     | 0.56              |
| 24:AY:92:ILE:HG23  | 24:AY:93:GLU:N     | 2.20                     | 0.56              |
| 25:B0:10:THR:HG21  | 35:BA:2277:G:OP2   | 2.05                     | 0.56              |
| 35:BA:1068:G:N2    | 35:BA:1096:A:H5'   | 2.19                     | 0.56              |
| 35:BA:1114:G:H2'   | 35:BA:1115:G:H5'   | 1.86                     | 0.56              |
| 35:BA:1386:C:H2'   | 35:BA:1387:C:C6    | 2.40                     | 0.56              |
| 35:BA:1398:C:H2'   | 35:BA:1399:C:H6    | 1.70                     | 0.56              |
| 35:BA:2021:C:H4'   | 35:BA:2022:U:OP2   | 2.05                     | 0.56              |
| 35:BA:2428:G:H4'   | 35:BA:2429:G:O5'   | 2.06                     | 0.56              |
| 35:BA:537:C:H2'    | 35:BA:538:G:H8     | 1.69                     | 0.56              |
| 35:BA:621:A:C2'    | 35:BA:622:G:H5'    | 2.34                     | 0.56              |
| 35:BA:884:C:H41    | 35:BA:886:C:H42    | 1.51                     | 0.56              |
| 40:BF:167:ALA:CB   | 40:BF:173:VAL:HG11 | 2.25                     | 0.56              |
| 35:BA:2305:A:C4    | 41:BG:154:GLY:HA3  | 2.40                     | 0.56              |
| 44:BK:106:GLU:CA   | 44:BK:109:LYS:HD3  | 2.30                     | 0.56              |
| 48:BP:127:ALA:O    | 48:BP:148:LEU:HD11 | 2.05                     | 0.56              |
| 57:BY:39:VAL:HG12  | 57:BY:40:GLU:N     | 2.21                     | 0.56              |
| 1:CA:1057:G:N2     | 1:CA:1204:A:H1'    | 2.20                     | 0.56              |
| 2:CB:30:ARG:HG3    | 2:CB:31:TYR:CD2    | 2.40                     | 0.56              |
| 5:CE:36:ASP:OD2    | 5:CE:40:ARG:HB2    | 2.05                     | 0.56              |
| 8:CH:120:THR:HG23  | 8:CH:123:GLU:OE1   | 2.05                     | 0.56              |
| 13:CM:106:ASN:O    | 13:CM:107:ALA:HB3  | 2.05                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:CN:37:PHE:HE1   | 14:CN:53:LEU:HD22  | 1.70                     | 0.56              |
| 18:CR:25:THR:O     | 18:CR:25:THR:HG22  | 2.05                     | 0.56              |
| 18:CR:56:THR:O     | 18:CR:58:LEU:HD12  | 2.04                     | 0.56              |
| 23:CX:11:U:H2'     | 23:CX:11:U:O2      | 2.03                     | 0.56              |
| 24:CY:147:TRP:O    | 24:CY:151:ARG:HG3  | 2.06                     | 0.56              |
| 24:CY:191:ASP:C    | 24:CY:193:GLY:H    | 2.08                     | 0.56              |
| 24:CY:247:ARG:HD2  | 24:CY:278:ASP:O    | 2.05                     | 0.56              |
| 25:D0:49:LYS:O     | 25:D0:51:VAL:HG23  | 2.04                     | 0.56              |
| 26:D1:6:GLU:O      | 26:D1:7:ILE:HD12   | 2.05                     | 0.56              |
| 32:D7:28:ARG:HH11  | 32:D7:28:ARG:HG3   | 1.68                     | 0.56              |
| 34:D9:27:CYS:SG    | 34:D9:29:ASN:ND2   | 2.78                     | 0.56              |
| 34:D9:31:LYS:HD3   | 35:DA:2478:A:OP1   | 2.05                     | 0.56              |
| 35:DA:2649:U:O2'   | 35:DA:2650:U:H5'   | 2.04                     | 0.56              |
| 35:DA:710:G:H1     | 35:DA:721:C:H42    | 1.51                     | 0.56              |
| 37:DC:29:LEU:O     | 37:DC:30:VAL:C     | 2.43                     | 0.56              |
| 38:DD:218:ARG:HG3  | 38:DD:218:ARG:HH11 | 1.71                     | 0.56              |
| 42:DH:16:SER:HB2   | 42:DH:27:LYS:CB    | 2.34                     | 0.56              |
| 42:DH:45:VAL:HA    | 42:DH:50:VAL:HG22  | 1.87                     | 0.56              |
| 52:DT:11:GLU:H     | 52:DT:11:GLU:CD    | 2.08                     | 0.56              |
| 1:AA:624:C:H2'     | 1:AA:625:G:H8      | 1.69                     | 0.56              |
| 1:AA:675:A:O2'     | 1:AA:676:A:H5'     | 2.05                     | 0.56              |
| 6:AF:67:MET:SD     | 6:AF:75:LEU:HD22   | 2.46                     | 0.56              |
| 7:AG:43:PHE:O      | 7:AG:46:ALA:HB3    | 2.05                     | 0.56              |
| 10:AJ:90:LEU:N     | 10:AJ:91:PRO:HD3   | 2.19                     | 0.56              |
| 24:AY:614:GLU:HA   | 24:AY:617:MET:HB2  | 1.87                     | 0.56              |
| 31:B6:16:CYS:O     | 31:B6:17:LYS:HB2   | 2.06                     | 0.56              |
| 31:B6:54:ILE:O     | 31:B6:54:ILE:CD1   | 2.52                     | 0.56              |
| 35:BA:1035:U:H2'   | 35:BA:1036:G:H8    | 1.68                     | 0.56              |
| 35:BA:206:U:O2     | 35:BA:206:U:H2'    | 2.04                     | 0.56              |
| 35:BA:2171:A:H1'   | 35:BA:2172:U:C5    | 2.40                     | 0.56              |
| 35:BA:2272:U:H5''  | 35:BA:2273:A:OP1   | 2.04                     | 0.56              |
| 35:BA:2287:A:N6    | 35:BA:2344:U:N3    | 2.48                     | 0.56              |
| 35:BA:292:C:O2'    | 35:BA:293:U:H5'    | 2.05                     | 0.56              |
| 35:BA:492:A:H2'    | 35:BA:493:G:H5'    | 1.88                     | 0.56              |
| 35:BA:654(L):G:H2' | 35:BA:654(M):C:H4' | 1.88                     | 0.56              |
| 35:BA:676:A:H2     | 35:BA:802:A:H61    | 1.51                     | 0.56              |
| 35:BA:850:C:O2'    | 35:BA:851:U:H5'    | 2.05                     | 0.56              |
| 38:BD:201:HIS:O    | 38:BD:204:ILE:HG12 | 2.06                     | 0.56              |
| 39:BE:101:ARG:NE   | 39:BE:171:GLU:HB2  | 2.20                     | 0.56              |
| 41:BG:138:GLN:NE2  | 41:BG:149:VAL:HG23 | 2.20                     | 0.56              |
| 41:BG:18:GLU:OE2   | 41:BG:18:GLU:HA    | 2.06                     | 0.56              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 42:BH:16:SER:CB   | 42:BH:27:LYS:HB2   | 2.32                     | 0.56              |
| 42:BH:46:GLU:OE1  | 42:BH:51:ARG:HB2   | 2.05                     | 0.56              |
| 43:BJ:118:UNK:C   | 43:BJ:120:UNK:H    | 2.18                     | 0.56              |
| 46:BN:21:LYS:HD2  | 46:BN:26:LEU:HB3   | 1.86                     | 0.56              |
| 46:BN:45:ASN:N    | 46:BN:45:ASN:HD22  | 1.83                     | 0.56              |
| 48:BP:27:HIS:C    | 48:BP:27:HIS:CD2   | 2.77                     | 0.56              |
| 51:BS:36:TYR:N    | 51:BS:36:TYR:CD1   | 2.74                     | 0.56              |
| 51:BS:90:GLY:C    | 51:BS:92:TYR:H     | 2.08                     | 0.56              |
| 52:BT:42:ILE:HD13 | 52:BT:83:ILE:HD13  | 1.88                     | 0.56              |
| 53:BU:8:VAL:HG23  | 53:BU:11:ARG:HH21  | 1.70                     | 0.56              |
| 54:BV:98:GLU:OE2  | 54:BV:100:ARG:HD3  | 2.06                     | 0.56              |
| 56:BX:8:ILE:H     | 56:BX:8:ILE:CD1    | 2.16                     | 0.56              |
| 1:CA:1226:C:H5'   | 13:CM:103:THR:CB   | 2.35                     | 0.56              |
| 1:CA:1422:G:O2'   | 1:CA:1423:G:H5'    | 2.05                     | 0.56              |
| 2:CB:153:ARG:C    | 2:CB:155:LEU:N     | 2.58                     | 0.56              |
| 18:CR:40:LEU:O    | 18:CR:42:ARG:N     | 2.38                     | 0.56              |
| 19:CS:48:THR:HG22 | 19:CS:61:TYR:HA    | 1.87                     | 0.56              |
| 22:CV:69:C:O2'    | 22:CV:70:G:H5'     | 2.05                     | 0.56              |
| 24:CY:409:ILE:CD1 | 24:CY:656:ALA:HB3  | 2.34                     | 0.56              |
| 24:CY:86:GLY:O    | 24:CY:88:VAL:HG22  | 2.04                     | 0.56              |
| 27:D2:69:ARG:CG   | 27:D2:70:GLN:N     | 2.64                     | 0.56              |
| 28:D3:9:VAL:HG11  | 28:D3:55:ARG:HD3   | 1.86                     | 0.56              |
| 35:DA:1336:A:H2'  | 35:DA:1337:G:C8    | 2.39                     | 0.56              |
| 35:DA:1336:A:P    | 56:DX:64:LYS:HE3   | 2.45                     | 0.56              |
| 35:DA:1662:C:H2'  | 35:DA:1663:C:C6    | 2.39                     | 0.56              |
| 35:DA:322:A:H5'   | 35:DA:340:A:H1'    | 1.87                     | 0.56              |
| 35:DA:881:G:H2'   | 35:DA:882:G:H5'    | 1.86                     | 0.56              |
| 35:DA:2051:A:H4'  | 39:DE:141:ILE:CD1  | 2.35                     | 0.56              |
| 41:DG:77:ILE:HG22 | 41:DG:80:PHE:H     | 1.70                     | 0.56              |
| 42:DH:105:LEU:H   | 42:DH:105:LEU:HD23 | 1.69                     | 0.56              |
| 46:DN:97:ARG:O    | 46:DN:101:HIS:HB2  | 2.05                     | 0.56              |
| 46:DN:58:ASP:C    | 46:DN:60:ILE:N     | 2.58                     | 0.56              |
| 49:DQ:55:VAL:HG13 | 49:DQ:56:ARG:N     | 2.19                     | 0.56              |
| 49:DQ:66:ILE:O    | 49:DQ:66:ILE:HG13  | 2.04                     | 0.56              |
| 53:DU:66:ASN:ND2  | 53:DU:76:TYR:H     | 2.04                     | 0.56              |
| 53:DU:65:ILE:HD11 | 53:DU:93:LYS:HA    | 1.87                     | 0.56              |
| 54:DV:82:ARG:HD2  | 54:DV:82:ARG:N     | 2.20                     | 0.56              |
| 56:DX:65:ARG:HH11 | 56:DX:65:ARG:HG2   | 1.70                     | 0.56              |
| 57:DY:2:ARG:N     | 57:DY:4:LYS:HG2    | 2.20                     | 0.56              |
| 57:DY:8:LYS:H     | 57:DY:8:LYS:HD2    | 1.68                     | 0.56              |
| 7:AG:38:LEU:O     | 7:AG:41:ARG:HB2    | 2.06                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:AJ:30:SER:HA    | 10:AJ:80:LYS:HE2   | 1.86                     | 0.56              |
| 18:AR:69:THR:O     | 18:AR:72:ARG:N     | 2.39                     | 0.56              |
| 19:AS:5:LEU:HG     | 19:AS:10:PHE:CD1   | 2.40                     | 0.56              |
| 19:AS:46:GLY:O     | 19:AS:48:THR:N     | 2.39                     | 0.56              |
| 24:AY:343:ASN:ND2  | 24:AY:343:ASN:C    | 2.59                     | 0.56              |
| 24:AY:496:LYS:HE2  | 24:AY:498:ILE:HD13 | 1.87                     | 0.56              |
| 24:AY:609:GLU:HA   | 24:AY:643:ILE:O    | 2.05                     | 0.56              |
| 24:AY:652:MET:O    | 24:AY:652:MET:HG3  | 2.04                     | 0.56              |
| 24:AY:655:TYR:HD2  | 24:AY:669:PHE:CE2  | 2.24                     | 0.56              |
| 29:B4:12:ALA:HB1   | 29:B4:29:PRO:HA    | 1.86                     | 0.56              |
| 31:B6:48:VAL:O     | 31:B6:49:HIS:HB2   | 2.05                     | 0.56              |
| 35:BA:1305:C:O2'   | 35:BA:1306:C:H5'   | 2.05                     | 0.56              |
| 35:BA:551:G:H2'    | 35:BA:552:G:H5'    | 1.87                     | 0.56              |
| 35:BA:680:G:H2'    | 35:BA:681:G:C8     | 2.40                     | 0.56              |
| 35:BA:58:G:H1      | 35:BA:69:C:H42     | 1.51                     | 0.56              |
| 38:BD:72:LYS:HB3   | 38:BD:75:ILE:HB    | 1.88                     | 0.56              |
| 39:BE:8:LYS:HG2    | 39:BE:192:ASN:HA   | 1.85                     | 0.56              |
| 43:BJ:54:UNK:O     | 43:BJ:56:UNK:N     | 2.38                     | 0.56              |
| 1:AA:1423:G:H5'    | 47:BO:49:ARG:HH22  | 1.69                     | 0.56              |
| 48:BP:7:ARG:HA     | 48:BP:7:ARG:CZ     | 2.35                     | 0.56              |
| 35:BA:2334:G:C4    | 51:BS:15:ARG:HD3   | 2.41                     | 0.56              |
| 53:BU:62:ILE:HG23  | 53:BU:76:TYR:CE1   | 2.40                     | 0.56              |
| 49:BQ:135:ASP:CG   | 58:BZ:49:ARG:NH1   | 2.58                     | 0.56              |
| 1:CA:1444:C:H2'    | 1:CA:1445:C:H6     | 1.67                     | 0.56              |
| 1:CA:67:C:H2'      | 1:CA:68:G:C8       | 2.40                     | 0.56              |
| 2:CB:60:ASP:O      | 2:CB:64:ARG:NH2    | 2.39                     | 0.56              |
| 18:CR:37:VAL:C     | 18:CR:39:VAL:H     | 2.08                     | 0.56              |
| 24:CY:209:ALA:O    | 24:CY:210:ARG:C    | 2.43                     | 0.56              |
| 24:CY:227:ILE:O    | 24:CY:227:ILE:HG22 | 2.05                     | 0.56              |
| 24:CY:33:LEU:HD12  | 24:CY:36:THR:HG21  | 1.86                     | 0.56              |
| 24:CY:488:THR:HG23 | 24:CY:600:VAL:HB   | 1.88                     | 0.56              |
| 26:D1:35:THR:HG23  | 26:D1:35:THR:O     | 2.04                     | 0.56              |
| 26:D1:7:ILE:CG2    | 26:D1:66:HIS:HD2   | 2.18                     | 0.56              |
| 30:D5:58:LEU:HD13  | 30:D5:59:GLU:N     | 2.20                     | 0.56              |
| 31:D6:37:ARG:NH2   | 35:DA:2286:A:N6    | 2.52                     | 0.56              |
| 35:DA:491:G:H2'    | 35:DA:492:A:C8     | 2.41                     | 0.56              |
| 35:DA:860:U:H5     | 35:DA:917:A:N7     | 2.03                     | 0.56              |
| 35:DA:947:G:H2'    | 35:DA:948:G:C8     | 2.40                     | 0.56              |
| 37:DC:14:LYS:HD3   | 37:DC:14:LYS:H     | 1.71                     | 0.56              |
| 38:DD:131:LEU:CD1  | 38:DD:131:LEU:N    | 2.66                     | 0.56              |
| 38:DD:26:LYS:HE2   | 38:DD:26:LYS:CA    | 2.35                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:DD:34:VAL:CG2   | 38:DD:35:LYS:H     | 2.02                     | 0.56              |
| 40:DF:119:ARG:HH11 | 40:DF:119:ARG:HG2  | 1.68                     | 0.56              |
| 40:DF:185:ASP:HA   | 40:DF:188:ARG:CD   | 2.34                     | 0.56              |
| 41:DG:5:VAL:HG12   | 41:DG:7:LEU:H      | 1.71                     | 0.56              |
| 42:DH:19:VAL:O     | 42:DH:20:ALA:HB2   | 2.05                     | 0.56              |
| 51:DS:88:ASP:OD2   | 51:DS:89:ARG:N     | 2.39                     | 0.56              |
| 35:DA:481:G:OP2    | 57:DY:47:LYS:HD3   | 2.05                     | 0.56              |
| 58:DZ:97:GLU:HA    | 58:DZ:126:VAL:O    | 2.06                     | 0.56              |
| 2:AB:114:ARG:HD2   | 2:AB:118:LEU:HG    | 1.86                     | 0.56              |
| 2:AB:215:LEU:O     | 2:AB:219:VAL:HG23  | 2.04                     | 0.56              |
| 2:AB:223:ILE:C     | 2:AB:225:ALA:H     | 2.07                     | 0.56              |
| 3:AC:112:SER:HB3   | 3:AC:115:LEU:HD12  | 1.86                     | 0.56              |
| 6:AF:4:TYR:CE1     | 6:AF:92:LYS:HD2    | 2.40                     | 0.56              |
| 8:AH:109:ILE:HG12  | 8:AH:110:ALA:H     | 1.70                     | 0.56              |
| 10:AJ:18:ALA:C     | 10:AJ:20:ALA:H     | 2.08                     | 0.56              |
| 10:AJ:90:LEU:N     | 10:AJ:91:PRO:CD    | 2.69                     | 0.56              |
| 14:AN:47:LEU:O     | 14:AN:50:LYS:N     | 2.39                     | 0.56              |
| 22:AW:74:A:C2'     | 22:AW:75:C:H5''    | 2.36                     | 0.56              |
| 24:AY:309:LEU:HD12 | 24:AY:310:ALA:N    | 2.20                     | 0.56              |
| 24:AY:534:ILE:HD11 | 24:AY:570:GLY:HA3  | 1.88                     | 0.56              |
| 26:B1:26:ARG:HG3   | 26:B1:27:GLU:HG3   | 1.86                     | 0.56              |
| 31:B6:9:LEU:HD12   | 31:B6:28:ARG:HG3   | 1.86                     | 0.56              |
| 33:B8:33:ASN:N     | 33:B8:36:LYS:HD2   | 2.20                     | 0.56              |
| 35:BA:1272:A:OP2   | 35:BA:1647:G:OP1   | 2.23                     | 0.56              |
| 35:BA:2030:A:H5''  | 35:BA:2031:A:OP1   | 2.05                     | 0.56              |
| 35:BA:573:G:O2'    | 35:BA:574:C:H3'    | 2.05                     | 0.56              |
| 37:BC:29:LEU:O     | 37:BC:30:VAL:C     | 2.43                     | 0.56              |
| 38:BD:112:GLN:H    | 38:BD:115:GLN:NE2  | 2.03                     | 0.56              |
| 40:BF:157:VAL:HG12 | 40:BF:176:LEU:HD23 | 1.87                     | 0.56              |
| 40:BF:160:ASN:HD22 | 40:BF:161:GLU:N    | 2.04                     | 0.56              |
| 40:BF:185:ASP:HA   | 40:BF:188:ARG:CG   | 2.34                     | 0.56              |
| 44:BK:93:ARG:HG3   | 58:BZ:112:ARG:NE   | 2.19                     | 0.56              |
| 48:BP:23:PRO:C     | 48:BP:33:ARG:CZ    | 2.73                     | 0.56              |
| 48:BP:55:ARG:CG    | 48:BP:56:SER:N     | 2.60                     | 0.56              |
| 56:BX:10:ALA:HB1   | 56:BX:11:PRO:HD2   | 1.87                     | 0.56              |
| 57:BY:25:GLY:HA3   | 57:BY:39:VAL:CG1   | 2.35                     | 0.56              |
| 1:CA:1133:G:N2     | 1:CA:1143:G:H1'    | 2.19                     | 0.56              |
| 1:CA:631:G:H8      | 1:CA:631:G:H5'     | 1.71                     | 0.56              |
| 1:CA:807:A:H2'     | 1:CA:808:C:C6      | 2.40                     | 0.56              |
| 4:CD:57:ARG:H      | 4:CD:57:ARG:HD2    | 1.69                     | 0.56              |
| 7:CG:51:GLN:HA     | 7:CG:51:GLN:OE1    | 2.06                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 12:CL:110:VAL:HG21  | 12:CL:120:TYR:HD2  | 1.70                     | 0.56              |
| 15:CO:9:GLN:HB3     | 15:CO:13:GLN:NE2   | 2.20                     | 0.56              |
| 24:CY:251:ILE:HG23  | 24:CY:281:PRO:HB3  | 1.87                     | 0.56              |
| 24:CY:366:VAL:HG23  | 24:CY:367:GLU:N    | 2.20                     | 0.56              |
| 29:D4:8:LYS:O       | 29:D4:9:LEU:CB     | 2.53                     | 0.56              |
| 31:D6:40:CYS:HB2    | 31:D6:46:HIS:ND1   | 2.20                     | 0.56              |
| 35:DA:1404:C:O2'    | 35:DA:1405:U:H5'   | 2.04                     | 0.56              |
| 35:DA:1948:G:H5'    | 35:DA:1948:G:H8    | 1.68                     | 0.56              |
| 35:DA:2011:U:H2'    | 35:DA:2012:G:H5'   | 1.87                     | 0.56              |
| 35:DA:614(A):U:H5'' | 35:DA:614(B):G:OP1 | 2.05                     | 0.56              |
| 35:DA:654(G):C:H2'  | 35:DA:654(H):G:C8  | 2.38                     | 0.56              |
| 35:DA:797:C:H2'     | 35:DA:798:G:H8     | 1.71                     | 0.56              |
| 35:DA:676:A:H2      | 35:DA:802:A:H61    | 1.53                     | 0.56              |
| 35:DA:848:G:H5''    | 35:DA:928:G:H22    | 1.69                     | 0.56              |
| 38:DD:166:GLN:HE21  | 38:DD:166:GLN:CA   | 2.18                     | 0.56              |
| 39:DE:95:ILE:HD13   | 39:DE:95:ILE:N     | 2.21                     | 0.56              |
| 41:DG:153:ARG:NH1   | 41:DG:153:ARG:HB3  | 2.20                     | 0.56              |
| 46:DN:87:LEU:HD21   | 46:DN:98:VAL:HG13  | 1.88                     | 0.56              |
| 48:DP:12:ALA:HB1    | 48:DP:16:ARG:HB3   | 1.87                     | 0.56              |
| 50:DR:11:ASN:O      | 50:DR:12:ARG:HB2   | 2.06                     | 0.56              |
| 35:DA:2334:G:C4     | 51:DS:15:ARG:HD3   | 2.40                     | 0.56              |
| 51:DS:30:ARG:NH2    | 51:DS:62:LYS:HD2   | 2.20                     | 0.56              |
| 52:DT:33:LYS:HE2    | 52:DT:43:GLN:CD    | 2.26                     | 0.56              |
| 1:AA:821:G:O2'      | 1:AA:822:C:H5'     | 2.05                     | 0.56              |
| 2:AB:178:ARG:HB2    | 2:AB:178:ARG:HH11  | 1.71                     | 0.56              |
| 2:AB:11:LEU:HD11    | 2:AB:217:ARG:NH2   | 2.20                     | 0.56              |
| 2:AB:44:LEU:HA      | 2:AB:47:THR:OG1    | 2.05                     | 0.56              |
| 4:AD:8:VAL:HB       | 4:AD:21:LEU:CD1    | 2.35                     | 0.56              |
| 5:AE:12:LEU:HD13    | 5:AE:12:LEU:C      | 2.25                     | 0.56              |
| 20:AT:49:ALA:CB     | 20:AT:99:LEU:HG    | 2.35                     | 0.56              |
| 35:BA:1185:C:H5'    | 35:BA:1186:G:P     | 2.46                     | 0.56              |
| 35:BA:1336:A:H2'    | 35:BA:1337:G:C8    | 2.40                     | 0.56              |
| 35:BA:1461:G:O2'    | 35:BA:1462:C:H5'   | 2.06                     | 0.56              |
| 35:BA:2026:C:N3     | 35:BA:2027:G:C8    | 2.74                     | 0.56              |
| 35:BA:455:C:N3      | 35:BA:472:A:H2'    | 2.21                     | 0.56              |
| 40:BF:25:PRO:CG     | 40:BF:119:ARG:HB2  | 2.35                     | 0.56              |
| 52:BT:53:ARG:HH11   | 52:BT:53:ARG:CB    | 2.17                     | 0.56              |
| 1:CA:1288:A:H2'     | 1:CA:1289:A:C8     | 2.39                     | 0.56              |
| 2:CB:51:LEU:HD23    | 2:CB:201:ILE:HD12  | 1.88                     | 0.56              |
| 12:CL:70:ILE:HG21   | 12:CL:77:LEU:CD1   | 2.35                     | 0.56              |
| 13:CM:49:THR:O      | 13:CM:53:VAL:HG23  | 2.06                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:D1:50:ARG:HG3  | 26:D1:59:THR:HG22  | 1.88                     | 0.56              |
| 26:D1:7:ILE:HG22  | 26:D1:66:HIS:CD2   | 2.34                     | 0.56              |
| 31:D6:11:LEU:CG   | 31:D6:26:ASN:HD21  | 2.17                     | 0.56              |
| 31:D6:15:GLU:HB2  | 31:D6:47:THR:HG21  | 1.87                     | 0.56              |
| 33:D8:14:VAL:HG21 | 33:D8:22:VAL:CG1   | 2.35                     | 0.56              |
| 35:DA:674:G:H2'   | 35:DA:804:A:H61    | 1.71                     | 0.56              |
| 35:DA:828:U:C5    | 35:DA:829:A:N6     | 2.74                     | 0.56              |
| 35:DA:845:G:OP2   | 35:DA:845:G:H8     | 1.88                     | 0.56              |
| 37:DC:95:VAL:HG12 | 37:DC:96:GLY:N     | 2.21                     | 0.56              |
| 39:DE:77:ILE:HG22 | 39:DE:78:LEU:HD12  | 1.86                     | 0.56              |
| 42:DH:46:GLU:OE1  | 42:DH:51:ARG:HB2   | 2.06                     | 0.56              |
| 46:DN:7:LYS:O     | 46:DN:9:VAL:N      | 2.38                     | 0.56              |
| 48:DP:50:ARG:O    | 48:DP:57:THR:HG22  | 2.06                     | 0.56              |
| 49:DQ:45:GLN:H    | 49:DQ:45:GLN:CD    | 2.01                     | 0.56              |
| 50:DR:7:GLY:C     | 50:DR:8:ARG:NE     | 2.59                     | 0.56              |
| 53:DU:106:PHE:O   | 53:DU:109:LEU:N    | 2.39                     | 0.56              |
| 57:DY:17:SER:HB2  | 57:DY:71:LYS:HD2   | 1.86                     | 0.56              |
| 1:AA:1130:A:C2    | 1:AA:1146:A:C4     | 2.94                     | 0.56              |
| 2:AB:119:GLU:OE1  | 2:AB:153:ARG:NH2   | 2.38                     | 0.56              |
| 2:AB:54:THR:HG22  | 2:AB:58:ILE:HD11   | 1.87                     | 0.56              |
| 5:AE:80:ILE:HG22  | 8:AH:104:ARG:HH22  | 1.66                     | 0.56              |
| 7:AG:27:ILE:HD11  | 7:AG:40:ALA:HA     | 1.87                     | 0.56              |
| 9:AI:79:LEU:CD1   | 9:AI:83:ARG:HD2    | 2.35                     | 0.56              |
| 18:AR:25:THR:O    | 18:AR:25:THR:HG22  | 2.05                     | 0.56              |
| 23:AX:13:A:C2'    | 23:AX:14:A:H5''    | 2.35                     | 0.56              |
| 24:AY:526:VAL:HB  | 24:AY:566:THR:HG23 | 1.88                     | 0.56              |
| 22:AV:2:G:H5''    | 25:B0:8:GLY:HA2    | 1.88                     | 0.56              |
| 28:B3:9:VAL:HG11  | 28:B3:55:ARG:HD3   | 1.88                     | 0.56              |
| 35:BA:406:G:O2'   | 35:BA:407:G:C8     | 2.58                     | 0.56              |
| 35:BA:933:A:H2'   | 35:BA:934:G:O4'    | 2.06                     | 0.56              |
| 35:BA:1774:C:O2   | 38:BD:11:PRO:HB2   | 2.05                     | 0.56              |
| 38:BD:161:THR:O   | 38:BD:162:SER:HB3  | 2.06                     | 0.56              |
| 35:BA:1567:A:H2'  | 38:BD:84:TYR:CE2   | 2.39                     | 0.56              |
| 39:BE:82:ARG:HG3  | 39:BE:83:ASP:H     | 1.70                     | 0.56              |
| 39:BE:89:ASP:O    | 39:BE:90:THR:O     | 2.23                     | 0.56              |
| 42:BH:159:GLU:OE1 | 42:BH:159:GLU:HA   | 2.06                     | 0.56              |
| 44:BK:58:THR:HB   | 44:BK:66:THR:CG2   | 2.35                     | 0.56              |
| 46:BN:126:PRO:O   | 46:BN:127:ASP:HB2  | 2.04                     | 0.56              |
| 46:BN:43:THR:HB   | 46:BN:46:VAL:HG11  | 1.86                     | 0.56              |
| 48:BP:127:ALA:HB3 | 48:BP:130:PHE:CZ   | 2.41                     | 0.56              |
| 50:BR:44:LEU:O    | 50:BR:44:LEU:HD13  | 2.04                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1442(B):A:N7  | 52:BT:118:ARG:HG2  | 2.20                     | 0.56              |
| 1:CA:1318:A:H2'    | 1:CA:1319:A:H5'    | 1.87                     | 0.56              |
| 1:CA:45:U:H2'      | 1:CA:46:G:H8       | 1.70                     | 0.56              |
| 2:CB:12:GLU:HA     | 2:CB:16:HIS:CG     | 2.40                     | 0.56              |
| 3:CC:119:ARG:O     | 3:CC:123:GLN:HG3   | 2.06                     | 0.56              |
| 4:CD:162:LEU:CD1   | 4:CD:181:MET:HG2   | 2.35                     | 0.56              |
| 5:CE:79:GLU:HB3    | 5:CE:92:LYS:HA     | 1.88                     | 0.56              |
| 6:CF:10:LEU:HD12   | 6:CF:61:LEU:HD13   | 1.88                     | 0.56              |
| 13:CM:77:ASN:O     | 13:CM:80:ARG:N     | 2.35                     | 0.56              |
| 24:CY:357:ARG:HG3  | 24:CY:366:VAL:HG11 | 1.86                     | 0.56              |
| 31:D6:43:CYS:HB2   | 31:D6:44:ARG:NH2   | 2.18                     | 0.56              |
| 35:DA:1220:A:H3'   | 35:DA:1221:C:C5'   | 2.36                     | 0.56              |
| 35:DA:1306:C:H2'   | 35:DA:1307:A:H8    | 1.70                     | 0.56              |
| 35:DA:1506:C:H2'   | 35:DA:1506:C:O2    | 2.06                     | 0.56              |
| 35:DA:2028:U:H2'   | 35:DA:2029:G:C8    | 2.41                     | 0.56              |
| 35:DA:2415:G:H4'   | 48:DP:67:MET:N     | 2.19                     | 0.56              |
| 35:DA:2681:C:H5    | 35:DA:2725:A:H62   | 1.53                     | 0.56              |
| 35:DA:2888:C:H2'   | 35:DA:2889:C:H6    | 1.70                     | 0.56              |
| 35:DA:551:G:H2'    | 35:DA:552:G:H5'    | 1.88                     | 0.56              |
| 40:DF:174:VAL:HG21 | 40:DF:189:THR:HG21 | 1.88                     | 0.56              |
| 40:DF:114:VAL:HG21 | 40:DF:202:PHE:CE1  | 2.40                     | 0.56              |
| 41:DG:138:GLN:O    | 41:DG:144:ILE:HD13 | 2.05                     | 0.56              |
| 42:DH:155:SER:O    | 42:DH:157:TYR:N    | 2.38                     | 0.56              |
| 46:DN:120:LEU:HD11 | 46:DN:122:VAL:HG23 | 1.86                     | 0.56              |
| 52:DT:106:SER:O    | 52:DT:107:ASP:CB   | 2.53                     | 0.56              |
| 52:DT:80:SER:CB    | 52:DT:81:PRO:CD    | 2.84                     | 0.56              |
| 53:DU:65:ILE:HG12  | 53:DU:96:ALA:HB1   | 1.88                     | 0.56              |
| 1:AA:1009:G:N3     | 1:AA:1009:G:H2'    | 2.20                     | 0.56              |
| 1:AA:1198:G:H2'    | 1:AA:1199:U:O4'    | 2.05                     | 0.56              |
| 1:AA:164:U:H2'     | 1:AA:165:C:C6      | 2.40                     | 0.56              |
| 2:AB:194:PRO:HG2   | 2:AB:195:ASP:H     | 1.71                     | 0.56              |
| 6:AF:91:VAL:HG12   | 6:AF:92:LYS:N      | 2.21                     | 0.56              |
| 10:AJ:47:PHE:CZ    | 14:AN:37:PHE:CE2   | 2.92                     | 0.56              |
| 17:AQ:99:SER:C     | 17:AQ:100:LYS:HG3  | 2.26                     | 0.56              |
| 1:AA:192:U:O4'     | 20:AT:103:GLY:HA2  | 2.06                     | 0.56              |
| 24:AY:446:THR:HG23 | 24:AY:448:GLN:HG2  | 1.88                     | 0.56              |
| 26:B1:58:ILE:HD11  | 26:B1:91:LYS:CA    | 2.36                     | 0.56              |
| 32:B7:35:ARG:HH11  | 32:B7:35:ARG:HG2   | 1.70                     | 0.56              |
| 35:BA:1306:C:H2'   | 35:BA:1307:A:H8    | 1.70                     | 0.56              |
| 35:BA:503:A:H4'    | 35:BA:504:U:C5'    | 2.36                     | 0.56              |
| 35:BA:82:G:H5''    | 35:BA:296:C:C5'    | 2.35                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:BC:95:VAL:HG12  | 37:BC:96:GLY:N     | 2.21                     | 0.56              |
| 41:BG:34:LEU:HD12  | 41:BG:34:LEU:N     | 2.21                     | 0.56              |
| 46:BN:24:GLY:HA2   | 46:BN:27:ALA:HB3   | 1.88                     | 0.56              |
| 48:BP:45:LEU:HG    | 48:BP:46:LYS:H     | 1.70                     | 0.56              |
| 52:BT:1:MET:H2     | 52:BT:7:ILE:HD11   | 1.67                     | 0.56              |
| 53:BU:65:ILE:HD11  | 53:BU:93:LYS:HA    | 1.88                     | 0.56              |
| 54:BV:38:LEU:H     | 54:BV:51:VAL:HG13  | 1.71                     | 0.56              |
| 55:BW:20:VAL:HG23  | 55:BW:47:VAL:HG21  | 1.88                     | 0.56              |
| 58:BZ:155:LEU:HD23 | 58:BZ:155:LEU:N    | 2.19                     | 0.56              |
| 1:CA:658:G:O4'     | 15:CO:22:THR:HB    | 2.06                     | 0.56              |
| 2:CB:7:VAL:O       | 2:CB:11:LEU:HG     | 2.05                     | 0.56              |
| 4:CD:132:ARG:HD2   | 4:CD:132:ARG:O     | 2.05                     | 0.56              |
| 12:CL:6:THR:OG1    | 12:CL:9:GLN:HG3    | 2.06                     | 0.56              |
| 18:CR:44:LEU:CD2   | 18:CR:79:LEU:HD22  | 2.36                     | 0.56              |
| 20:CT:24:LEU:HD13  | 20:CT:24:LEU:O     | 2.05                     | 0.56              |
| 24:CY:238:THR:C    | 24:CY:240:GLU:N    | 2.59                     | 0.56              |
| 24:CY:498:ILE:HG22 | 24:CY:507:TYR:CD2  | 2.41                     | 0.56              |
| 31:D6:27:LYS:HB3   | 31:D6:30:THR:HG22  | 1.87                     | 0.56              |
| 31:D6:7:ILE:HD12   | 31:D6:7:ILE:N      | 2.20                     | 0.56              |
| 35:DA:2272:U:H5''  | 35:DA:2273:A:OP1   | 2.05                     | 0.56              |
| 35:DA:2512:C:H2'   | 35:DA:2513:G:O4'   | 2.05                     | 0.56              |
| 26:D1:81:LYS:NZ    | 35:DA:271(H):G:H4' | 2.20                     | 0.56              |
| 35:DA:688:U:H4'    | 35:DA:1780:A:C2    | 2.41                     | 0.56              |
| 42:DH:12:PRO:O     | 42:DH:15:VAL:HG22  | 2.04                     | 0.56              |
| 42:DH:173:PRO:C    | 42:DH:175:LYS:H    | 2.08                     | 0.56              |
| 43:DJ:130:UNK:O    | 43:DJ:132:UNK:N    | 2.39                     | 0.56              |
| 45:DL:81:UNK:O     | 45:DL:82:UNK:O     | 2.22                     | 0.56              |
| 48:DP:16:ARG:HB2   | 48:DP:16:ARG:HH11  | 1.69                     | 0.56              |
| 48:DP:7:ARG:HA     | 48:DP:7:ARG:CZ     | 2.36                     | 0.56              |
| 54:DV:54:GLY:O     | 54:DV:55:ALA:HB2   | 2.05                     | 0.56              |
| 54:DV:98:GLU:OE2   | 54:DV:100:ARG:HD3  | 2.06                     | 0.56              |
| 57:DY:17:SER:CB    | 57:DY:71:LYS:HD2   | 2.36                     | 0.56              |
| 57:DY:59:GLY:O     | 57:DY:60:PHE:HB2   | 2.06                     | 0.56              |
| 58:DZ:10:ARG:HB3   | 58:DZ:36:LYS:CB    | 2.35                     | 0.56              |
| 1:AA:728:A:H2'     | 1:AA:729:A:C8      | 2.41                     | 0.56              |
| 1:AA:973:G:C1'     | 10:AJ:55:LYS:CE    | 2.83                     | 0.56              |
| 2:AB:153:ARG:C     | 2:AB:155:LEU:N     | 2.57                     | 0.56              |
| 2:AB:238:LEU:O     | 2:AB:238:LEU:HG    | 2.06                     | 0.56              |
| 4:AD:57:ARG:H      | 4:AD:57:ARG:HD2    | 1.70                     | 0.56              |
| 5:AE:76:ILE:HG13   | 5:AE:77:PRO:HD2    | 1.88                     | 0.56              |
| 13:AM:10:PRO:HG3   | 13:AM:18:ALA:HB1   | 1.87                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:AW:60:A:C2'     | 22:AW:61:U:H5'     | 2.36                     | 0.56              |
| 24:AY:119:GLU:O    | 24:AY:120:THR:OG1  | 2.24                     | 0.56              |
| 24:AY:381:LYS:HD2  | 24:AY:381:LYS:N    | 2.20                     | 0.56              |
| 35:BA:1290:C:H2'   | 35:BA:1291:C:H6    | 1.71                     | 0.56              |
| 35:BA:1678:G:H22   | 35:BA:1989:G:H22   | 1.53                     | 0.56              |
| 25:B0:43:THR:HG22  | 35:BA:2331:G:O2'   | 2.05                     | 0.56              |
| 35:BA:2415:G:H4'   | 48:BP:67:MET:N     | 2.20                     | 0.56              |
| 35:BA:2583:G:H2'   | 35:BA:2584:U:O2    | 2.05                     | 0.56              |
| 35:BA:2804:C:H2'   | 35:BA:2805:G:H8    | 1.71                     | 0.56              |
| 35:BA:751:A:C5'    | 55:BW:90:ARG:HA    | 2.35                     | 0.56              |
| 35:BA:986:C:O2'    | 35:BA:987:G:H5'    | 2.06                     | 0.56              |
| 36:BB:22:U:H2'     | 36:BB:23:G:C8      | 2.41                     | 0.56              |
| 37:BC:215:VAL:HG23 | 37:BC:225:ILE:HG12 | 1.86                     | 0.56              |
| 40:BF:2:LYS:HG3    | 40:BF:25:PRO:HG2   | 1.86                     | 0.56              |
| 41:BG:31:VAL:HG22  | 41:BG:32:PRO:HD2   | 1.87                     | 0.56              |
| 41:BG:7:LEU:O      | 41:BG:11:TYR:N     | 2.37                     | 0.56              |
| 35:BA:2657:A:O2'   | 42:BH:160:LYS:HE3  | 2.05                     | 0.56              |
| 42:BH:86:GLU:HB2   | 42:BH:132:ARG:HB3  | 1.87                     | 0.56              |
| 48:BP:50:ARG:O     | 48:BP:57:THR:HG22  | 2.06                     | 0.56              |
| 51:BS:88:ASP:CG    | 51:BS:89:ARG:H     | 2.07                     | 0.56              |
| 51:BS:88:ASP:OD2   | 51:BS:89:ARG:N     | 2.39                     | 0.56              |
| 35:BA:583:G:OP2    | 53:BU:10:ARG:HD2   | 2.06                     | 0.56              |
| 54:BV:51:VAL:HG12  | 54:BV:52:VAL:N     | 2.14                     | 0.56              |
| 1:CA:255:G:O6      | 1:CA:266:G:O6      | 2.24                     | 0.56              |
| 2:CB:194:PRO:HG2   | 2:CB:195:ASP:H     | 1.70                     | 0.56              |
| 2:CB:21:ARG:HB3    | 2:CB:39:ILE:HA     | 1.87                     | 0.56              |
| 7:CG:91:VAL:HG12   | 7:CG:92:SER:N      | 2.21                     | 0.56              |
| 9:CI:79:LEU:CD1    | 9:CI:83:ARG:HB2    | 2.34                     | 0.56              |
| 11:CK:108:ILE:N    | 11:CK:108:ILE:CD1  | 2.69                     | 0.56              |
| 13:CM:81:LEU:HB3   | 13:CM:89:GLY:HA2   | 1.87                     | 0.56              |
| 17:CQ:80:GLY:O     | 17:CQ:81:ARG:HD2   | 2.06                     | 0.56              |
| 24:CY:206:LEU:CD1  | 24:CY:210:ARG:HH12 | 2.19                     | 0.56              |
| 24:CY:227:ILE:HD11 | 24:CY:241:GLU:O    | 2.05                     | 0.56              |
| 25:D0:20:ARG:CD    | 25:D0:20:ARG:H     | 2.19                     | 0.56              |
| 29:D4:9:LEU:CD1    | 29:D4:10:VAL:H     | 2.19                     | 0.56              |
| 34:D9:29:ASN:HD21  | 34:D9:32:HIS:CG    | 2.23                     | 0.56              |
| 35:DA:1149:G:H2'   | 35:DA:1150:C:C6    | 2.41                     | 0.56              |
| 35:DA:2103:C:H2'   | 35:DA:2103:C:O2    | 2.04                     | 0.56              |
| 35:DA:2110:G:HO2'  | 35:DA:2120:G:H5'   | 1.68                     | 0.56              |
| 35:DA:933:A:H2'    | 35:DA:934:G:O4'    | 2.06                     | 0.56              |
| 39:DE:82:ARG:HG3   | 39:DE:83:ASP:H     | 1.71                     | 0.56              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:DJ:26:UNK:HA    | 43:DJ:84:UNK:CA    | 2.35                     | 0.56              |
| 44:DK:24:GLY:H     | 44:DK:25:PRO:HD2   | 1.69                     | 0.56              |
| 49:DQ:97:VAL:HG11  | 49:DQ:103:MET:HE3  | 1.88                     | 0.56              |
| 54:DV:18:LEU:CD1   | 54:DV:19:LYS:H     | 2.18                     | 0.56              |
| 1:AA:1142:G:H2'    | 1:AA:1143:G:O4'    | 2.06                     | 0.56              |
| 1:AA:1499:A:H1'    | 1:AA:1520:G:H5'    | 1.88                     | 0.56              |
| 1:AA:807:A:H2'     | 1:AA:808:C:C6      | 2.41                     | 0.56              |
| 3:AC:46:GLU:HB3    | 3:AC:83:ARG:HH22   | 1.71                     | 0.56              |
| 5:AE:101:ILE:O     | 5:AE:101:ILE:HG12  | 2.06                     | 0.56              |
| 6:AF:37:VAL:CG1    | 6:AF:38:GLU:H      | 2.12                     | 0.56              |
| 11:AK:12:ARG:O     | 11:AK:13:GLN:HG3   | 2.05                     | 0.56              |
| 24:AY:77:HIS:NE2   | 24:AY:277:VAL:HG21 | 2.21                     | 0.56              |
| 24:AY:415:PRO:O    | 24:AY:420:ASP:HB2  | 2.05                     | 0.56              |
| 24:AY:539:ILE:O    | 24:AY:542:VAL:HG12 | 2.06                     | 0.56              |
| 35:BA:2103:C:H2'   | 35:BA:2103:C:O2    | 2.06                     | 0.56              |
| 35:BA:2746:U:O2'   | 35:BA:2747:G:H5'   | 2.06                     | 0.56              |
| 35:BA:2845:G:O2'   | 35:BA:2846:G:H5'   | 2.06                     | 0.56              |
| 35:BA:438:G:O2'    | 35:BA:440:G:H5'    | 2.05                     | 0.56              |
| 40:BF:40:GLN:OE1   | 40:BF:184:TYR:HB2  | 2.06                     | 0.56              |
| 41:BG:36:LYS:HA    | 41:BG:99:MET:SD    | 2.46                     | 0.56              |
| 47:BO:52:VAL:O     | 47:BO:53:LYS:HG3   | 2.06                     | 0.56              |
| 30:B5:55:ARG:HH12  | 50:BR:33:ARG:CD    | 2.19                     | 0.56              |
| 50:BR:21:TYR:HB3   | 50:BR:47:PHE:CE2   | 2.41                     | 0.56              |
| 52:BT:120:ARG:HA   | 52:BT:123:GLN:HG2  | 1.88                     | 0.56              |
| 58:BZ:180:VAL:HG12 | 58:BZ:181:GLU:N    | 2.19                     | 0.56              |
| 58:BZ:53:ILE:HG22  | 58:BZ:71:VAL:HB    | 1.87                     | 0.56              |
| 1:CA:1142:G:H2'    | 1:CA:1143:G:O4'    | 2.06                     | 0.56              |
| 1:CA:1298:C:H1'    | 1:CA:1299:A:C6     | 2.41                     | 0.56              |
| 1:CA:1312:G:O2'    | 1:CA:1313:U:H5'    | 2.06                     | 0.56              |
| 1:CA:45:U:H2'      | 1:CA:46:G:C8       | 2.40                     | 0.56              |
| 1:CA:620:C:C2      | 4:CD:135:LEU:HG    | 2.41                     | 0.56              |
| 2:CB:119:GLU:OE1   | 2:CB:153:ARG:NH2   | 2.37                     | 0.56              |
| 2:CB:62:ALA:O      | 2:CB:64:ARG:N      | 2.35                     | 0.56              |
| 3:CC:77:ILE:HA     | 3:CC:84:ILE:HB     | 1.88                     | 0.56              |
| 4:CD:25:ARG:HH12   | 4:CD:30:LYS:HB2    | 1.71                     | 0.56              |
| 6:CF:52:ILE:O      | 6:CF:53:ALA:HB3    | 2.06                     | 0.56              |
| 7:CG:38:LEU:O      | 7:CG:42:ILE:HG13   | 2.06                     | 0.56              |
| 8:CH:10:LEU:CD2    | 8:CH:83:ILE:HD11   | 2.35                     | 0.56              |
| 10:CJ:96:ILE:N     | 10:CJ:96:ILE:HD13  | 2.20                     | 0.56              |
| 13:CM:10:PRO:HG3   | 13:CM:18:ALA:HB1   | 1.87                     | 0.56              |
| 13:CM:83:ASP:CG    | 13:CM:84:ILE:N     | 2.60                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:CO:39:LEU:CD1   | 15:CO:56:LEU:HB2   | 2.36                     | 0.56              |
| 24:CY:217:VAL:HA   | 24:CY:220:ALA:HB3  | 1.88                     | 0.56              |
| 24:CY:314:PHE:CE1  | 24:CY:327:PHE:HB3  | 2.41                     | 0.56              |
| 31:D6:53:LYS:HG3   | 31:D6:54:ILE:HG23  | 1.88                     | 0.56              |
| 35:DA:1185:C:H5'   | 35:DA:1186:G:P     | 2.45                     | 0.56              |
| 35:DA:1624:G:O2'   | 35:DA:1625:C:H5'   | 2.06                     | 0.56              |
| 35:DA:1692:U:H2'   | 35:DA:1694:C:C5    | 2.41                     | 0.56              |
| 35:DA:1847:A:H3'   | 35:DA:1848:A:C5'   | 2.36                     | 0.56              |
| 35:DA:192:C:C2'    | 35:DA:193:U:H5'    | 2.31                     | 0.56              |
| 35:DA:2132:U:C5    | 37:DC:6:LYS:HD2    | 2.41                     | 0.56              |
| 35:DA:877:U:O2'    | 35:DA:878:A:H5''   | 2.06                     | 0.56              |
| 36:DB:77:U:O2'     | 36:DB:78:A:H5'     | 2.06                     | 0.56              |
| 35:DA:1567:A:H2'   | 38:DD:84:TYR:CE2   | 2.40                     | 0.56              |
| 40:DF:157:VAL:HG22 | 40:DF:194:MET:HG2  | 1.87                     | 0.56              |
| 40:DF:195:ASP:CG   | 40:DF:196:LEU:H    | 2.07                     | 0.56              |
| 42:DH:140:LYS:O    | 42:DH:144:VAL:HG23 | 2.06                     | 0.56              |
| 44:DK:58:THR:HB    | 44:DK:66:THR:CG2   | 2.36                     | 0.56              |
| 48:DP:112:LEU:O    | 48:DP:128:HIS:HB2  | 2.06                     | 0.56              |
| 48:DP:27:HIS:CD2   | 48:DP:27:HIS:C     | 2.79                     | 0.56              |
| 49:DQ:2:LEU:O      | 49:DQ:3:MET:HB3    | 2.06                     | 0.56              |
| 58:DZ:35:ARG:CZ    | 58:DZ:35:ARG:HB3   | 2.36                     | 0.56              |
| 58:DZ:42:VAL:HG13  | 58:DZ:43:GLU:N     | 2.21                     | 0.56              |
| 58:DZ:43:GLU:O     | 58:DZ:47:VAL:HG23  | 2.06                     | 0.56              |
| 1:AA:1133:G:N2     | 1:AA:1143:G:H1'    | 2.18                     | 0.56              |
| 1:AA:1318:A:O3'    | 19:AS:10:PHE:CD2   | 2.59                     | 0.56              |
| 6:AF:52:ILE:O      | 6:AF:53:ALA:HB3    | 2.06                     | 0.56              |
| 24:AY:218:GLU:O    | 24:AY:221:ALA:HB3  | 2.06                     | 0.56              |
| 24:AY:438:PHE:C    | 24:AY:438:PHE:CD2  | 2.77                     | 0.56              |
| 31:B6:15:GLU:OE1   | 31:B6:44:ARG:NH2   | 2.39                     | 0.56              |
| 32:B7:24:THR:HG23  | 32:B7:27:GLY:HA3   | 1.87                     | 0.56              |
| 35:BA:2076:U:H5'   | 35:BA:2238:G:N2    | 2.20                     | 0.56              |
| 35:BA:2855:C:H2'   | 35:BA:2856:C:C6    | 2.41                     | 0.56              |
| 38:BD:76:PRO:HG2   | 38:BD:98:VAL:CG2   | 2.36                     | 0.56              |
| 40:BF:25:PRO:HG3   | 40:BF:119:ARG:CB   | 2.34                     | 0.56              |
| 41:BG:67:LYS:HD3   | 41:BG:68:PRO:CD    | 2.36                     | 0.56              |
| 41:BG:91:ARG:HD2   | 41:BG:92:VAL:CA    | 2.34                     | 0.56              |
| 42:BH:88:LEU:HD23  | 42:BH:164:TYR:O    | 2.06                     | 0.56              |
| 42:BH:86:GLU:HB3   | 42:BH:132:ARG:HB3  | 1.88                     | 0.56              |
| 52:BT:65:LYS:HZ2   | 52:BT:65:LYS:HA    | 1.67                     | 0.56              |
| 53:BU:26:GLY:O     | 53:BU:28:ARG:N     | 2.39                     | 0.56              |
| 58:BZ:136:PHE:CD1  | 58:BZ:136:PHE:O    | 2.59                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1009:G:H2'    | 1:CA:1009:G:N3     | 2.21                     | 0.56              |
| 1:CA:299:G:H2'     | 1:CA:300:A:H8      | 1.68                     | 0.56              |
| 1:CA:363:A:OP1     | 12:CL:33:ARG:HD3   | 2.06                     | 0.56              |
| 3:CC:79:ARG:HH11   | 3:CC:79:ARG:CB     | 2.12                     | 0.56              |
| 8:CH:103:VAL:HG12  | 8:CH:108:GLY:HA3   | 1.88                     | 0.56              |
| 24:CY:605:ILE:CG2  | 24:CY:646:PHE:HB3  | 2.35                     | 0.56              |
| 31:D6:11:LEU:HD23  | 31:D6:51:GLU:CG    | 2.36                     | 0.56              |
| 35:DA:1278:A:O2'   | 35:DA:1279:G:H5'   | 2.05                     | 0.56              |
| 35:DA:1332:G:N2    | 35:DA:1609:A:H3'   | 2.20                     | 0.56              |
| 35:DA:1505:C:C5    | 35:DA:1506:C:H1'   | 2.41                     | 0.56              |
| 25:D0:10:THR:HG21  | 35:DA:2277:G:OP2   | 2.06                     | 0.56              |
| 35:DA:246:C:H2'    | 35:DA:247:G:H5'    | 1.88                     | 0.56              |
| 35:DA:2754:U:H2'   | 35:DA:2755:C:H5'   | 1.87                     | 0.56              |
| 35:DA:884:C:H41    | 35:DA:886:C:H42    | 1.53                     | 0.56              |
| 37:DC:139:PRO:HA   | 37:DC:145:THR:HB   | 1.88                     | 0.56              |
| 37:DC:42:VAL:O     | 37:DC:176:VAL:HG22 | 2.06                     | 0.56              |
| 40:DF:152:GLU:O    | 40:DF:153:SER:C    | 2.44                     | 0.56              |
| 44:DK:86:LYS:NZ    | 44:DK:86:LYS:HB3   | 2.21                     | 0.56              |
| 46:DN:74:ARG:NH2   | 46:DN:83:LYS:HD3   | 2.20                     | 0.56              |
| 47:DO:115:VAL:CG1  | 47:DO:121:VAL:HG21 | 2.35                     | 0.56              |
| 48:DP:58:THR:C     | 48:DP:61:ARG:HE    | 2.06                     | 0.56              |
| 35:DA:2469:A:O3'   | 49:DQ:56:ARG:NH1   | 2.39                     | 0.56              |
| 52:DT:126:ALA:C    | 52:DT:128:GLU:H    | 2.08                     | 0.56              |
| 54:DV:52:VAL:O     | 54:DV:52:VAL:HG13  | 2.06                     | 0.56              |
| 1:AA:111:G:O6      | 1:AA:330:C:N4      | 2.39                     | 0.55              |
| 1:AA:680:C:O2'     | 1:AA:681:C:H5'     | 2.06                     | 0.55              |
| 2:AB:97:TRP:CZ2    | 2:AB:102:LEU:HD13  | 2.35                     | 0.55              |
| 4:AD:4:TYR:O       | 4:AD:5:ILE:CB      | 2.54                     | 0.55              |
| 6:AF:62:TRP:O      | 6:AF:63:TYR:CG     | 2.60                     | 0.55              |
| 7:AG:64:GLN:CG     | 7:AG:128:ALA:HB1   | 2.36                     | 0.55              |
| 11:AK:67:ASP:OD1   | 11:AK:71:LYS:HE3   | 2.06                     | 0.55              |
| 13:AM:81:LEU:HD22  | 13:AM:81:LEU:N     | 2.22                     | 0.55              |
| 15:AO:76:GLU:O     | 15:AO:78:TYR:N     | 2.39                     | 0.55              |
| 24:AY:165:GLN:HE21 | 24:AY:177:ILE:HG21 | 1.71                     | 0.55              |
| 24:AY:20:HIS:O     | 24:AY:21:ILE:O     | 2.24                     | 0.55              |
| 24:AY:622:GLY:O    | 24:AY:625:ASN:N    | 2.38                     | 0.55              |
| 24:AY:8:ASP:O      | 24:AY:9:LEU:HB3    | 2.06                     | 0.55              |
| 35:BA:1247:A:OP1   | 40:BF:95:ARG:NH2   | 2.38                     | 0.55              |
| 35:BA:1692:U:H2'   | 35:BA:1694:C:C5    | 2.41                     | 0.55              |
| 35:BA:1971:A:C4    | 38:BD:241:PRO:HD3  | 2.41                     | 0.55              |
| 35:BA:2107:C:H42   | 35:BA:2182:G:H1    | 1.54                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:BA:2769:C:O2'  | 35:BA:2770:G:H5'   | 2.06                     | 0.55              |
| 35:BA:709:U:H2'   | 35:BA:710:G:C8     | 2.42                     | 0.55              |
| 36:BB:114:C:H2'   | 36:BB:115:G:C8     | 2.41                     | 0.55              |
| 37:BC:97:GLY:O    | 37:BC:100:ILE:HG12 | 2.06                     | 0.55              |
| 35:BA:1654:A:H2   | 39:BE:113:PHE:CD1  | 2.24                     | 0.55              |
| 41:BG:29:TRP:C    | 41:BG:31:VAL:H     | 2.10                     | 0.55              |
| 42:BH:20:ALA:HB1  | 42:BH:21:PRO:HD2   | 1.88                     | 0.55              |
| 42:BH:83:TYR:O    | 42:BH:84:SER:HB3   | 2.05                     | 0.55              |
| 44:BK:86:LYS:HB3  | 44:BK:86:LYS:NZ    | 2.21                     | 0.55              |
| 49:BQ:27:VAL:HG21 | 49:BQ:134:ARG:HG2  | 1.88                     | 0.55              |
| 52:BT:132:LYS:HG2 | 52:BT:133:GLU:H    | 1.71                     | 0.55              |
| 53:BU:76:TYR:CD2  | 53:BU:76:TYR:C     | 2.79                     | 0.55              |
| 57:BY:86:ARG:HB3  | 57:BY:88:LYS:NZ    | 2.21                     | 0.55              |
| 58:BZ:103:ARG:HB2 | 58:BZ:136:PHE:HB2  | 1.87                     | 0.55              |
| 58:BZ:67:LEU:HD12 | 58:BZ:67:LEU:H     | 1.71                     | 0.55              |
| 58:BZ:67:LEU:N    | 58:BZ:67:LEU:HD12  | 2.21                     | 0.55              |
| 1:CA:1333:A:C2    | 1:CA:1334:G:H1'    | 2.41                     | 0.55              |
| 1:CA:192:U:O4'    | 20:CT:103:GLY:HA2  | 2.05                     | 0.55              |
| 6:CF:37:VAL:CG1   | 6:CF:38:GLU:H      | 2.09                     | 0.55              |
| 14:CN:44:LEU:HD12 | 14:CN:44:LEU:O     | 2.06                     | 0.55              |
| 19:CS:9:VAL:CG1   | 19:CS:9:VAL:O      | 2.54                     | 0.55              |
| 24:CY:389:LEU:N   | 24:CY:389:LEU:HD12 | 2.20                     | 0.55              |
| 27:D2:64:LEU:O    | 27:D2:68:ARG:HB2   | 2.06                     | 0.55              |
| 30:D5:46:CYS:SG   | 30:D5:47:PRO:HD2   | 2.46                     | 0.55              |
| 31:D6:27:LYS:NZ   | 31:D6:30:THR:HB    | 2.22                     | 0.55              |
| 35:DA:1036:G:C6   | 35:DA:1120:G:C6    | 2.94                     | 0.55              |
| 35:DA:2713:A:C3'  | 35:DA:2714:G:C5'   | 2.84                     | 0.55              |
| 26:D1:81:LYS:HZ2  | 35:DA:271(H):G:H4' | 1.71                     | 0.55              |
| 35:DA:892:G:H2'   | 35:DA:893:C:H6     | 1.71                     | 0.55              |
| 36:DB:20:C:H2'    | 36:DB:21:G:C5'     | 2.37                     | 0.55              |
| 35:DA:1796:U:OP1  | 38:DD:276:LYS:HE3  | 2.06                     | 0.55              |
| 44:DK:77:LEU:HD12 | 44:DK:107:ILE:CG2  | 2.31                     | 0.55              |
| 54:DV:49:THR:HB   | 54:DV:50:PRO:CD    | 2.36                     | 0.55              |
| 1:AA:1298:C:H1'   | 1:AA:1299:A:C6     | 2.41                     | 0.55              |
| 1:AA:1368:G:O2'   | 1:AA:1369:C:H5'    | 2.06                     | 0.55              |
| 1:AA:1347:G:N2    | 1:AA:1373:G:H2'    | 2.21                     | 0.55              |
| 1:AA:1381:U:C5    | 1:AA:1382:C:C5     | 2.94                     | 0.55              |
| 2:AB:189:ASP:O    | 2:AB:191:ASP:N     | 2.40                     | 0.55              |
| 3:AC:130:VAL:HG21 | 3:AC:157:ILE:HG23  | 1.88                     | 0.55              |
| 5:AE:79:GLU:HB3   | 5:AE:92:LYS:HA     | 1.88                     | 0.55              |
| 7:AG:12:LEU:CD1   | 7:AG:25:ALA:HB2    | 2.37                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 9:AI:73:GLN:O      | 9:AI:76:ALA:N     | 2.39                     | 0.55              |
| 13:AM:6:GLY:C      | 13:AM:8:GLU:N     | 2.59                     | 0.55              |
| 15:AO:74:ASP:OD2   | 15:AO:77:ARG:HG2  | 2.06                     | 0.55              |
| 22:AV:21:A:N6      | 22:AV:46:G:H2'    | 2.05                     | 0.55              |
| 22:AV:68:C:H2'     | 22:AV:69:C:C6     | 2.41                     | 0.55              |
| 24:AY:250:THR:O    | 24:AY:252:ASP:N   | 2.39                     | 0.55              |
| 27:B2:25:VAL:C     | 27:B2:27:GLU:N    | 2.59                     | 0.55              |
| 31:B6:15:GLU:CD    | 31:B6:44:ARG:NH2  | 2.60                     | 0.55              |
| 32:B7:28:ARG:HG3   | 32:B7:28:ARG:NH1  | 2.21                     | 0.55              |
| 35:BA:2050:C:O2'   | 35:BA:2051:A:H5'  | 2.07                     | 0.55              |
| 35:BA:363(B):G:H2' | 35:BA:363(C):G:C8 | 2.38                     | 0.55              |
| 35:BA:67:U:H2'     | 35:BA:68:G:H8     | 1.70                     | 0.55              |
| 35:BA:8:A:H2'      | 35:BA:9:U:C5      | 2.41                     | 0.55              |
| 44:BK:13:PRO:HA    | 44:BK:52:ILE:HG23 | 1.88                     | 0.55              |
| 48:BP:122:PRO:O    | 48:BP:123:LEU:HB3 | 2.07                     | 0.55              |
| 48:BP:47:ASP:CB    | 48:BP:51:PHE:HB2  | 2.36                     | 0.55              |
| 35:BA:2469:A:O3'   | 49:BQ:56:ARG:NH1  | 2.39                     | 0.55              |
| 53:BU:93:LYS:H     | 53:BU:93:LYS:HD2  | 1.72                     | 0.55              |
| 54:BV:19:LYS:NZ    | 54:BV:20:LEU:H    | 2.03                     | 0.55              |
| 56:BX:18:TYR:C     | 56:BX:20:GLY:N    | 2.59                     | 0.55              |
| 1:CA:1391:U:H2'    | 1:CA:1392:G:C8    | 2.41                     | 0.55              |
| 1:CA:741:G:O2'     | 1:CA:742:G:H5'    | 2.06                     | 0.55              |
| 6:CF:47:ARG:HG2    | 6:CF:47:ARG:HH11  | 1.71                     | 0.55              |
| 11:CK:48:ILE:HG22  | 11:CK:49:GLY:N    | 2.21                     | 0.55              |
| 27:D2:50:ILE:CG2   | 27:D2:54:LYS:HE3  | 2.36                     | 0.55              |
| 35:DA:1858:G:H2'   | 35:DA:1883:G:N2   | 2.21                     | 0.55              |
| 35:DA:2389:G:H5''  | 35:DA:2390:U:C5'  | 2.34                     | 0.55              |
| 35:DA:2428:G:H4'   | 35:DA:2429:G:O5'  | 2.06                     | 0.55              |
| 30:D5:7:PRO:HA     | 35:DA:2615:U:C2   | 2.41                     | 0.55              |
| 35:DA:274:G:N3     | 35:DA:274:G:H2'   | 2.19                     | 0.55              |
| 38:DD:241:PRO:O    | 38:DD:242:ARG:HB2 | 2.06                     | 0.55              |
| 38:DD:65:ILE:N     | 38:DD:65:ILE:HD13 | 2.21                     | 0.55              |
| 41:DG:141:PHE:HB2  | 41:DG:144:ILE:CG2 | 2.35                     | 0.55              |
| 44:DK:13:PRO:HA    | 44:DK:52:ILE:HG23 | 1.88                     | 0.55              |
| 52:DT:132:LYS:HG2  | 52:DT:133:GLU:N   | 2.21                     | 0.55              |
| 52:DT:26:ASP:C     | 52:DT:26:ASP:OD2  | 2.44                     | 0.55              |
| 57:DY:13:VAL:HG22  | 57:DY:73:ARG:O    | 2.06                     | 0.55              |
| 1:AA:1090:U:C4'    | 1:AA:1170:A:H2    | 2.19                     | 0.55              |
| 1:AA:1226:C:H5'    | 13:AM:96:LEU:CD1  | 2.36                     | 0.55              |
| 1:AA:1364:U:C2'    | 1:AA:1364:U:O2    | 2.49                     | 0.55              |
| 1:AA:1369:C:H2'    | 1:AA:1370:G:H8    | 1.71                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:AA:1392:G:H21    | 1:AA:1502:A:H8      | 1.53                     | 0.55              |
| 1:AA:505:G:H2'     | 1:AA:506:G:C8       | 2.41                     | 0.55              |
| 1:AA:52:G:O2'      | 1:AA:53:A:H5'       | 2.06                     | 0.55              |
| 1:AA:630:G:H2'     | 1:AA:631:G:H5''     | 1.85                     | 0.55              |
| 1:AA:973:G:H1'     | 10:AJ:55:LYS:HZ1    | 1.66                     | 0.55              |
| 1:AA:977:A:H2'     | 1:AA:978:A:H5'      | 1.89                     | 0.55              |
| 4:AD:61:LYS:CE     | 4:AD:62:GLN:HE21    | 2.19                     | 0.55              |
| 7:AG:91:VAL:HG12   | 7:AG:92:SER:N       | 2.20                     | 0.55              |
| 13:AM:121:LYS:HD3  | 13:AM:121:LYS:N     | 2.20                     | 0.55              |
| 24:AY:176:GLY:HA3  | 24:AY:187:THR:HA    | 1.89                     | 0.55              |
| 24:AY:230:LYS:HZ2  | 24:AY:230:LYS:HB2   | 1.72                     | 0.55              |
| 29:B4:8:LYS:O      | 29:B4:9:LEU:CB      | 2.54                     | 0.55              |
| 30:B5:33:CYS:SG    | 30:B5:36:CYS:SG     | 3.04                     | 0.55              |
| 30:B5:58:LEU:HD13  | 30:B5:59:GLU:N      | 2.22                     | 0.55              |
| 31:B6:43:CYS:HB2   | 31:B6:44:ARG:NH2    | 2.19                     | 0.55              |
| 35:BA:1149:G:H2'   | 35:BA:1150:C:C6     | 2.41                     | 0.55              |
| 35:BA:1220:A:H3'   | 35:BA:1221:C:C5'    | 2.36                     | 0.55              |
| 35:BA:1812:A:O2'   | 35:BA:1813:G:H5'    | 2.06                     | 0.55              |
| 35:BA:2688:U:H1'   | 35:BA:2721:A:N6     | 2.21                     | 0.55              |
| 35:BA:271(K):U:H3' | 35:BA:271(L):U:H5'' | 1.88                     | 0.55              |
| 35:BA:467:G:O2'    | 35:BA:468:G:H5'     | 2.05                     | 0.55              |
| 35:BA:483:A:H4'    | 57:BY:49:VAL:HA     | 1.88                     | 0.55              |
| 40:BF:75:HIS:HE1   | 40:BF:82:ILE:HD11   | 1.71                     | 0.55              |
| 42:BH:155:SER:O    | 42:BH:157:TYR:N     | 2.38                     | 0.55              |
| 42:BH:41:MET:O     | 42:BH:42:ARG:CB     | 2.54                     | 0.55              |
| 50:BR:103:ARG:HD2  | 55:BW:40:ASN:HD21   | 1.71                     | 0.55              |
| 52:BT:33:LYS:HE2   | 52:BT:43:GLN:CD     | 2.26                     | 0.55              |
| 35:BA:993:G:OP1    | 53:BU:50:ARG:HD2    | 2.05                     | 0.55              |
| 57:BY:84:ARG:NH1   | 57:BY:84:ARG:HG2    | 2.21                     | 0.55              |
| 58:BZ:119:GLU:C    | 58:BZ:121:HIS:H     | 2.09                     | 0.55              |
| 58:BZ:137:ILE:CG2  | 58:BZ:155:LEU:HD12  | 2.37                     | 0.55              |
| 1:CA:895:G:H5''    | 1:CA:896:C:OP2      | 2.07                     | 0.55              |
| 9:CI:7:THR:O       | 9:CI:83:ARG:HD2     | 2.05                     | 0.55              |
| 11:CK:12:ARG:O     | 11:CK:13:GLN:HG3    | 2.07                     | 0.55              |
| 1:CA:689:C:P       | 11:CK:46:GLY:HA3    | 2.47                     | 0.55              |
| 1:CA:1014:A:H4'    | 19:CS:14:HIS:ND1    | 2.20                     | 0.55              |
| 24:CY:658:ASP:O    | 24:CY:662:LYS:HG2   | 2.06                     | 0.55              |
| 26:D1:60:PHE:CD1   | 26:D1:91:LYS:HE3    | 2.42                     | 0.55              |
| 28:D3:5:LYS:HE3    | 28:D3:34:GLU:OE1    | 2.06                     | 0.55              |
| 32:D7:34:ARG:HH12  | 32:D7:39:ARG:HD2    | 1.71                     | 0.55              |
| 34:D9:19:ARG:HB2   | 35:DA:2756:U:H5'    | 1.87                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:2171:A:H1'   | 35:DA:2172:U:C5    | 2.40                     | 0.55              |
| 35:DA:2247:A:O2'   | 35:DA:2248:C:H5'   | 2.06                     | 0.55              |
| 35:DA:2815:C:H2'   | 35:DA:2816:C:H6    | 1.69                     | 0.55              |
| 35:DA:41:C:H2'     | 35:DA:42:G:O4'     | 2.07                     | 0.55              |
| 35:DA:687:C:H2'    | 35:DA:688:U:O4'    | 2.07                     | 0.55              |
| 35:DA:945:A:O2'    | 35:DA:946:G:H4'    | 2.06                     | 0.55              |
| 39:DE:49:LEU:N     | 39:DE:49:LEU:CD2   | 2.68                     | 0.55              |
| 40:DF:113:ALA:HB1  | 40:DF:186:ILE:CG2  | 2.34                     | 0.55              |
| 41:DG:86:MET:N     | 41:DG:87:PRO:CD    | 2.67                     | 0.55              |
| 24:CY:218:GLU:HG2  | 45:DL:84:UNK:CB    | 2.36                     | 0.55              |
| 48:DP:33:ARG:O     | 48:DP:34:GLY:C     | 2.43                     | 0.55              |
| 51:DS:59:LYS:CD    | 51:DS:61:ASN:HB2   | 2.35                     | 0.55              |
| 51:DS:90:GLY:C     | 51:DS:92:TYR:H     | 2.09                     | 0.55              |
| 58:DZ:139:VAL:HG12 | 58:DZ:141:VAL:HG23 | 1.88                     | 0.55              |
| 58:DZ:43:GLU:HG3   | 58:DZ:44:PHE:H     | 1.72                     | 0.55              |
| 58:DZ:59:LEU:O     | 58:DZ:66:SER:HA    | 2.06                     | 0.55              |
| 1:AA:1318:A:H2'    | 1:AA:1319:A:H5'    | 1.88                     | 0.55              |
| 1:AA:277:C:O2'     | 1:AA:278:G:H5'     | 2.06                     | 0.55              |
| 3:AC:136:GLN:C     | 3:AC:138:VAL:N     | 2.58                     | 0.55              |
| 3:AC:35:GLU:OE2    | 3:AC:59:ARG:NH1    | 2.39                     | 0.55              |
| 7:AG:121:ALA:O     | 7:AG:125:MET:HG3   | 2.07                     | 0.55              |
| 10:AJ:29:ARG:HH11  | 10:AJ:29:ARG:HG2   | 1.72                     | 0.55              |
| 1:AA:275:G:H5''    | 17:AQ:14:LYS:CB    | 2.34                     | 0.55              |
| 19:AS:43:GLU:HB2   | 19:AS:44:MET:SD    | 2.46                     | 0.55              |
| 22:AV:17:C:C6      | 22:AV:17(A):U:C5   | 2.92                     | 0.55              |
| 22:AW:16:C:H3'     | 22:AW:17:C:O2      | 2.06                     | 0.55              |
| 24:AY:252:ASP:OD2  | 24:AY:252:ASP:N    | 2.39                     | 0.55              |
| 24:AY:417:THR:O    | 24:AY:419:ALA:N    | 2.40                     | 0.55              |
| 24:AY:553:GLY:HA2  | 24:AY:560:VAL:HG23 | 1.89                     | 0.55              |
| 24:AY:624:LEU:HD11 | 24:AY:655:TYR:OH   | 2.06                     | 0.55              |
| 24:AY:662:LYS:HZ2  | 42:BH:175:LYS:HD2  | 1.71                     | 0.55              |
| 34:B9:31:LYS:HD3   | 35:BA:2478:A:OP1   | 2.06                     | 0.55              |
| 35:BA:1115:G:H2'   | 35:BA:1116:C:C6    | 2.41                     | 0.55              |
| 35:BA:1141:U:H5''  | 46:BN:63:THR:HG23  | 1.88                     | 0.55              |
| 35:BA:1751:C:O2'   | 35:BA:1752:C:H5'   | 2.07                     | 0.55              |
| 35:BA:2170:A:H5''  | 37:BC:135:ARG:HH21 | 1.70                     | 0.55              |
| 35:BA:252:G:O2'    | 35:BA:253:C:H5'    | 2.06                     | 0.55              |
| 35:BA:2562:U:H1'   | 47:BO:23:ARG:NH1   | 2.16                     | 0.55              |
| 35:BA:2657:A:H2'   | 35:BA:2658:C:C5'   | 2.37                     | 0.55              |
| 35:BA:2713:A:C3'   | 35:BA:2714:G:C5'   | 2.84                     | 0.55              |
| 35:BA:55:G:H2'     | 35:BA:56:A:C8      | 2.41                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:962:G:H2'    | 35:BA:963:U:O4'    | 2.07                     | 0.55              |
| 36:BB:20:C:H2'     | 36:BB:21:G:C5'     | 2.36                     | 0.55              |
| 39:BE:34:VAL:HG11  | 39:BE:78:LEU:CD2   | 2.37                     | 0.55              |
| 40:BF:174:VAL:HG21 | 40:BF:189:THR:HG21 | 1.88                     | 0.55              |
| 41:BG:38:VAL:HG22  | 41:BG:93:THR:HG23  | 1.89                     | 0.55              |
| 52:BT:25:GLY:HA2   | 52:BT:92:GLY:HA2   | 1.87                     | 0.55              |
| 54:BV:49:THR:HB    | 54:BV:50:PRO:CD    | 2.37                     | 0.55              |
| 30:B5:27:PRO:CG    | 55:BW:23:LEU:HD11  | 2.35                     | 0.55              |
| 57:BY:13:VAL:O     | 57:BY:24:VAL:HA    | 2.07                     | 0.55              |
| 57:BY:39:VAL:HG12  | 57:BY:40:GLU:HG2   | 1.88                     | 0.55              |
| 58:BZ:115:GLY:HA2  | 58:BZ:177:PRO:HG3  | 1.88                     | 0.55              |
| 58:BZ:14:LYS:O     | 58:BZ:18:LEU:HD13  | 2.06                     | 0.55              |
| 1:CA:1431:C:H2'    | 1:CA:1432:G:O4'    | 2.06                     | 0.55              |
| 1:CA:505:G:H2'     | 1:CA:506:G:C8      | 2.41                     | 0.55              |
| 4:CD:159:ARG:HH11  | 4:CD:159:ARG:HG3   | 1.71                     | 0.55              |
| 5:CE:91:LEU:HD13   | 5:CE:120:THR:HG22  | 1.87                     | 0.55              |
| 5:CE:36:ASP:O      | 5:CE:37:ARG:CB     | 2.55                     | 0.55              |
| 10:CJ:18:ALA:O     | 10:CJ:20:ALA:N     | 2.36                     | 0.55              |
| 19:CS:46:GLY:O     | 19:CS:48:THR:N     | 2.39                     | 0.55              |
| 35:DA:1151:G:H5''  | 53:DU:81:HIS:CE1   | 2.41                     | 0.55              |
| 35:DA:1491:G:N2    | 35:DA:1492:G:H1'   | 2.21                     | 0.55              |
| 35:DA:510:C:OP1    | 35:DA:510:C:H3'    | 2.05                     | 0.55              |
| 35:DA:67:U:H2'     | 35:DA:68:G:H8      | 1.71                     | 0.55              |
| 35:DA:936:C:H2'    | 35:DA:937:U:H6     | 1.70                     | 0.55              |
| 36:DB:22:U:H2'     | 36:DB:23:G:C8      | 2.42                     | 0.55              |
| 38:DD:259:THR:O    | 38:DD:260:ARG:C    | 2.43                     | 0.55              |
| 38:DD:26:LYS:HE2   | 38:DD:26:LYS:HA    | 1.87                     | 0.55              |
| 40:DF:157:VAL:HG22 | 40:DF:194:MET:HA   | 1.88                     | 0.55              |
| 35:DA:1084:A:OP1   | 43:DJ:55:UNK:HA    | 2.07                     | 0.55              |
| 44:DK:112:MET:N    | 44:DK:113:PRO:HD2  | 2.20                     | 0.55              |
| 52:DT:132:LYS:HG2  | 52:DT:133:GLU:H    | 1.71                     | 0.55              |
| 52:DT:85:LYS:HZ2   | 52:DT:85:LYS:HB3   | 1.68                     | 0.55              |
| 54:DV:39:LEU:HD22  | 54:DV:39:LEU:N     | 2.22                     | 0.55              |
| 50:DR:103:ARG:HD2  | 55:DW:40:ASN:HD21  | 1.71                     | 0.55              |
| 58:DZ:17:ALA:CA    | 58:DZ:20:ARG:HG2   | 2.36                     | 0.55              |
| 1:AA:1116:C:H2'    | 1:AA:1117:G:C5'    | 2.35                     | 0.55              |
| 1:AA:663:A:O2'     | 1:AA:664:G:H5'     | 2.07                     | 0.55              |
| 1:AA:759:A:H2'     | 1:AA:760:G:H5'     | 1.87                     | 0.55              |
| 2:AB:97:TRP:CH2    | 2:AB:173:ALA:HA    | 2.41                     | 0.55              |
| 3:AC:154:SER:OG    | 3:AC:155:GLY:N     | 2.40                     | 0.55              |
| 4:AD:9:CYS:HB3     | 4:AD:32:ALA:HB2    | 1.89                     | 0.55              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:942:G:H21     | 9:AI:124:GLN:HE22  | 1.52                     | 0.55              |
| 9:AI:3:GLN:NE2     | 9:AI:20:ARG:NH2    | 2.55                     | 0.55              |
| 12:AL:47:LYS:HB3   | 12:AL:47:LYS:HZ2   | 1.70                     | 0.55              |
| 12:AL:70:ILE:HG21  | 12:AL:77:LEU:CD1   | 2.37                     | 0.55              |
| 17:AQ:44:ALA:HA    | 17:AQ:71:PHE:O     | 2.07                     | 0.55              |
| 27:B2:20:GLU:HG3   | 27:B2:21:LEU:N     | 2.22                     | 0.55              |
| 29:B4:48:ARG:O     | 29:B4:49:PHE:CD1   | 2.59                     | 0.55              |
| 31:B6:15:GLU:OE2   | 31:B6:44:ARG:CZ    | 2.55                     | 0.55              |
| 34:B9:4:ARG:HH12   | 35:BA:2477:C:N4    | 2.04                     | 0.55              |
| 35:BA:271(E):U:H2' | 35:BA:271(F):C:C6  | 2.42                     | 0.55              |
| 35:BA:82:G:C5'     | 35:BA:296:C:H5'    | 2.35                     | 0.55              |
| 38:BD:176:ARG:CG   | 38:BD:176:ARG:HH11 | 2.19                     | 0.55              |
| 39:BE:38:THR:CB    | 39:BE:41:LYS:HG2   | 2.34                     | 0.55              |
| 40:BF:114:VAL:HG21 | 40:BF:202:PHE:CE1  | 2.40                     | 0.55              |
| 40:BF:185:ASP:HA   | 40:BF:188:ARG:CD   | 2.36                     | 0.55              |
| 35:BA:674:G:C1'    | 40:BF:74:ARG:HD3   | 2.37                     | 0.55              |
| 35:BA:1258:C:O4'   | 40:BF:84:VAL:HG21  | 2.06                     | 0.55              |
| 43:BJ:13:UNK:C     | 43:BJ:15:UNK:N     | 2.66                     | 0.55              |
| 47:BO:47:ILE:O     | 47:BO:48:PRO:O     | 2.24                     | 0.55              |
| 48:BP:66:GLY:O     | 48:BP:67:MET:HB3   | 2.06                     | 0.55              |
| 57:BY:3:VAL:HG12   | 57:BY:3:VAL:O      | 2.07                     | 0.55              |
| 57:BY:90:LEU:HD12  | 57:BY:91:GLU:OE2   | 2.05                     | 0.55              |
| 36:BB:104:U:O3'    | 58:BZ:72:ARG:NH1   | 2.39                     | 0.55              |
| 1:CA:1113:C:H2'    | 1:CA:1114:C:H6     | 1.71                     | 0.55              |
| 1:CA:651:C:H2'     | 1:CA:652:U:C6      | 2.41                     | 0.55              |
| 1:CA:728:A:H2'     | 1:CA:729:A:C8      | 2.42                     | 0.55              |
| 2:CB:235:SER:O     | 2:CB:237:ALA:N     | 2.29                     | 0.55              |
| 2:CB:97:TRP:CH2    | 2:CB:173:ALA:HA    | 2.41                     | 0.55              |
| 3:CC:164:ARG:NH2   | 3:CC:166:GLU:OE1   | 2.39                     | 0.55              |
| 3:CC:167:TRP:O     | 3:CC:168:ALA:HB3   | 2.06                     | 0.55              |
| 5:CE:107:ARG:HG2   | 5:CE:108:ALA:N     | 2.19                     | 0.55              |
| 6:CF:60:PHE:C      | 6:CF:61:LEU:HD12   | 2.27                     | 0.55              |
| 10:CJ:29:ARG:HH11  | 10:CJ:29:ARG:HG2   | 1.72                     | 0.55              |
| 10:CJ:56:HIS:O     | 10:CJ:58:ASP:N     | 2.40                     | 0.55              |
| 12:CL:25:PRO:C     | 12:CL:27:LEU:N     | 2.57                     | 0.55              |
| 13:CM:116:THR:HG22 | 13:CM:117:VAL:N    | 2.20                     | 0.55              |
| 19:CS:53:ASN:C     | 19:CS:55:LYS:H     | 2.10                     | 0.55              |
| 20:CT:26:ASN:O     | 20:CT:30:LYS:HB2   | 2.07                     | 0.55              |
| 24:CY:182:ARG:O    | 24:CY:184:LYS:N    | 2.40                     | 0.55              |
| 25:D0:25:ARG:HD2   | 25:D0:29:GLN:HE21  | 1.71                     | 0.55              |
| 35:DA:120:U:O2'    | 35:DA:149:A:C8     | 2.56                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:1678:G:H22   | 35:DA:1989:G:H22   | 1.50                     | 0.55              |
| 35:DA:2291:U:H2'   | 35:DA:2292:C:H6    | 1.68                     | 0.55              |
| 35:DA:250:G:H2'    | 35:DA:251:A:C8     | 2.42                     | 0.55              |
| 35:DA:941:A:H4'    | 48:DP:35:HIS:HE1   | 1.71                     | 0.55              |
| 37:DC:128:LEU:CD2  | 37:DC:132:LEU:HD12 | 2.37                     | 0.55              |
| 38:DD:146:GLU:HB2  | 38:DD:189:CYS:HB3  | 1.88                     | 0.55              |
| 39:DE:133:LYS:C    | 39:DE:134:ILE:HG13 | 2.27                     | 0.55              |
| 39:DE:93:VAL:HG12  | 39:DE:175:VAL:HG21 | 1.89                     | 0.55              |
| 40:DF:206:ILE:HG22 | 40:DF:207:GLY:N    | 2.22                     | 0.55              |
| 35:DA:675:A:OP1    | 40:DF:63:LYS:HE2   | 2.06                     | 0.55              |
| 40:DF:69:HIS:CD2   | 40:DF:69:HIS:N     | 2.73                     | 0.55              |
| 48:DP:112:LEU:H    | 48:DP:128:HIS:CD2  | 2.24                     | 0.55              |
| 48:DP:47:ASP:HB2   | 48:DP:51:PHE:HB2   | 1.89                     | 0.55              |
| 49:DQ:116:GLU:O    | 49:DQ:120:ILE:HG12 | 2.06                     | 0.55              |
| 50:DR:83:ILE:O     | 50:DR:87:TYR:HE2   | 1.89                     | 0.55              |
| 57:DY:13:VAL:O     | 57:DY:24:VAL:HA    | 2.06                     | 0.55              |
| 57:DY:3:VAL:O      | 57:DY:3:VAL:HG12   | 2.06                     | 0.55              |
| 58:DZ:10:ARG:CD    | 58:DZ:36:LYS:HE2   | 2.24                     | 0.55              |
| 1:AA:1015:A:H2'    | 1:AA:1016:A:O4'    | 2.07                     | 0.55              |
| 1:AA:1342:C:H1'    | 9:AI:124:GLN:HG3   | 1.88                     | 0.55              |
| 4:AD:26:CYS:O      | 4:AD:31:CYS:HB2    | 2.07                     | 0.55              |
| 9:AI:82:ALA:HA     | 9:AI:85:LEU:HD11   | 1.89                     | 0.55              |
| 11:AK:122:LYS:O    | 11:AK:123:LYS:C    | 2.44                     | 0.55              |
| 12:AL:111:LYS:O    | 12:AL:112:ASP:HB2  | 2.06                     | 0.55              |
| 13:AM:33:ALA:HA    | 13:AM:59:TYR:HE2   | 1.70                     | 0.55              |
| 24:AY:150:ILE:C    | 24:AY:152:THR:H    | 2.10                     | 0.55              |
| 24:AY:390:VAL:HG23 | 24:AY:391:GLY:O    | 2.07                     | 0.55              |
| 24:AY:528:ALA:HB3  | 24:AY:567:LEU:O    | 2.07                     | 0.55              |
| 26:B1:18:ILE:CD1   | 26:B1:37:ILE:HG12  | 2.36                     | 0.55              |
| 31:B6:27:LYS:NZ    | 31:B6:30:THR:HB    | 2.21                     | 0.55              |
| 33:B8:23:VAL:CG1   | 33:B8:46:ARG:HH11  | 2.19                     | 0.55              |
| 35:BA:271(F):C:O2' | 35:BA:271(G):C:H5' | 2.06                     | 0.55              |
| 35:BA:28:A:H62     | 35:BA:512:G:H1'    | 1.72                     | 0.55              |
| 35:BA:624:C:H41    | 48:BP:107:LYS:HZ3  | 1.55                     | 0.55              |
| 35:BA:705:A:N1     | 35:BA:727:A:H1'    | 2.22                     | 0.55              |
| 35:BA:790:C:H5'    | 35:BA:791:C:OP2    | 2.07                     | 0.55              |
| 40:BF:157:VAL:HG22 | 40:BF:194:MET:HA   | 1.89                     | 0.55              |
| 41:BG:49:ASP:O     | 41:BG:50:ALA:HB3   | 2.06                     | 0.55              |
| 42:BH:124:GLU:CG   | 42:BH:132:ARG:HG3  | 2.36                     | 0.55              |
| 47:BO:115:VAL:CG1  | 47:BO:121:VAL:HG21 | 2.37                     | 0.55              |
| 47:BO:60:ALA:HA    | 47:BO:87:ILE:HD13  | 1.89                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:BP:48:PRO:O    | 48:BP:50:ARG:N     | 2.39                     | 0.55              |
| 49:BQ:97:VAL:HG11 | 49:BQ:103:MET:HE3  | 1.87                     | 0.55              |
| 51:BS:49:VAL:HG21 | 51:BS:77:ALA:HB2   | 1.88                     | 0.55              |
| 53:BU:66:ASN:ND2  | 53:BU:76:TYR:H     | 2.05                     | 0.55              |
| 54:BV:54:GLY:O    | 54:BV:55:ALA:HB2   | 2.07                     | 0.55              |
| 49:BQ:59:ARG:CA   | 58:BZ:180:VAL:HG23 | 2.35                     | 0.55              |
| 1:CA:1294:G:C2'   | 1:CA:1295:G:H5'    | 2.36                     | 0.55              |
| 1:CA:261:U:H2'    | 1:CA:263:A:OP2     | 2.06                     | 0.55              |
| 1:CA:93:G:O2'     | 1:CA:96:U:H5'      | 2.05                     | 0.55              |
| 3:CC:126:ARG:HB2  | 3:CC:128:PHE:CE2   | 2.41                     | 0.55              |
| 3:CC:62:ASP:O     | 3:CC:64:VAL:HG23   | 2.06                     | 0.55              |
| 4:CD:12:CYS:SG    | 4:CD:19:LEU:O      | 2.64                     | 0.55              |
| 16:CP:74:LEU:O    | 16:CP:79:VAL:HG23  | 2.07                     | 0.55              |
| 19:CS:5:LEU:HG    | 19:CS:10:PHE:CD1   | 2.41                     | 0.55              |
| 24:CY:77:HIS:CD2  | 24:CY:277:VAL:HG21 | 2.41                     | 0.55              |
| 24:CY:649:LEU:CD2 | 24:CY:671:MET:HE3  | 2.37                     | 0.55              |
| 30:D5:50:GLY:HA2  | 30:D5:56:LYS:HB3   | 1.88                     | 0.55              |
| 31:D6:9:LEU:HD12  | 31:D6:28:ARG:CG    | 2.36                     | 0.55              |
| 33:D8:23:VAL:CG1  | 33:D8:46:ARG:HH11  | 2.19                     | 0.55              |
| 35:DA:1477:A:H5'  | 35:DA:1478:G:OP2   | 2.07                     | 0.55              |
| 35:DA:1539:G:H2'  | 35:DA:1540:U:O4'   | 2.07                     | 0.55              |
| 35:DA:1669:A:H2'  | 35:DA:1670:C:H5'   | 1.88                     | 0.55              |
| 35:DA:1910:G:O2'  | 35:DA:1911:U:H5'   | 2.05                     | 0.55              |
| 30:D5:3:LYS:HG2   | 35:DA:747:U:O4     | 2.06                     | 0.55              |
| 35:DA:82:G:H5''   | 35:DA:296:C:C5'    | 2.33                     | 0.55              |
| 35:DA:883:G:O2'   | 35:DA:884:C:H5'    | 2.07                     | 0.55              |
| 36:DB:7:G:C3'     | 36:DB:8:U:H5''     | 2.36                     | 0.55              |
| 39:DE:34:VAL:HG12 | 39:DE:48:GLN:O     | 2.06                     | 0.55              |
| 40:DF:7:TYR:HD2   | 40:DF:16:GLY:CA    | 2.14                     | 0.55              |
| 41:DG:18:GLU:OE2  | 41:DG:18:GLU:HA    | 2.06                     | 0.55              |
| 41:DG:37:VAL:O    | 41:DG:94:LEU:HB2   | 2.07                     | 0.55              |
| 42:DH:173:PRO:O   | 42:DH:175:LYS:N    | 2.40                     | 0.55              |
| 47:DO:63:VAL:O    | 47:DO:64:ARG:HG2   | 2.07                     | 0.55              |
| 35:DA:958:U:H5'   | 49:DQ:14:ARG:NH1   | 2.21                     | 0.55              |
| 52:DT:55:ASN:HD22 | 52:DT:58:ASN:ND2   | 2.04                     | 0.55              |
| 54:DV:66:ARG:CZ   | 54:DV:88:ARG:HH21  | 2.19                     | 0.55              |
| 57:DY:13:VAL:HG22 | 57:DY:14:LEU:H     | 1.71                     | 0.55              |
| 1:AA:936:C:O2'    | 1:AA:937:A:H5'     | 2.07                     | 0.55              |
| 2:AB:12:GLU:HA    | 2:AB:16:HIS:CG     | 2.42                     | 0.55              |
| 2:AB:193:ASP:OD2  | 2:AB:193:ASP:O     | 2.25                     | 0.55              |
| 3:AC:126:ARG:HB2  | 3:AC:128:PHE:CE2   | 2.42                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:AE:79:GLU:HB3    | 5:AE:93:PRO:HD2    | 1.89                     | 0.55              |
| 7:AG:64:GLN:HG3    | 7:AG:128:ALA:HB1   | 1.88                     | 0.55              |
| 9:AI:7:THR:O       | 9:AI:83:ARG:HD2    | 2.07                     | 0.55              |
| 1:AA:1308:U:H5''   | 13:AM:98:VAL:CG2   | 2.35                     | 0.55              |
| 24:AY:406:GLU:HB3  | 24:AY:407:PRO:CD   | 2.35                     | 0.55              |
| 24:AY:687:LEU:O    | 24:AY:689:LYS:N    | 2.40                     | 0.55              |
| 26:B1:68:PRO:O     | 26:B1:70:VAL:N     | 2.39                     | 0.55              |
| 27:B2:38:GLN:C     | 27:B2:40:SER:H     | 2.10                     | 0.55              |
| 33:B8:47:LYS:HZ3   | 33:B8:49:VAL:HG13  | 1.72                     | 0.55              |
| 35:BA:1156:A:C2'   | 35:BA:1157:G:OP1   | 2.55                     | 0.55              |
| 35:BA:1573:G:H2'   | 35:BA:1574:C:H5'   | 1.89                     | 0.55              |
| 35:BA:2247:A:O2'   | 35:BA:2248:C:H5'   | 2.06                     | 0.55              |
| 35:BA:2543:G:N3    | 35:BA:2765:A:H2'   | 2.22                     | 0.55              |
| 30:B5:3:LYS:NZ     | 35:BA:2613:U:C2'   | 2.70                     | 0.55              |
| 37:BC:92:ALA:HB2   | 37:BC:154:ILE:HD13 | 1.87                     | 0.55              |
| 38:BD:241:PRO:O    | 38:BD:242:ARG:CB   | 2.54                     | 0.55              |
| 39:BE:77:ILE:HG22  | 39:BE:78:LEU:HD12  | 1.89                     | 0.55              |
| 41:BG:109:VAL:HG11 | 41:BG:142:PRO:HD3  | 1.88                     | 0.55              |
| 48:BP:102:ARG:CB   | 48:BP:102:ARG:NH2  | 2.69                     | 0.55              |
| 48:BP:67:MET:O     | 48:BP:68:GLN:HG3   | 2.07                     | 0.55              |
| 51:BS:36:TYR:O     | 51:BS:37:ALA:HB2   | 2.07                     | 0.55              |
| 53:BU:59:ARG:O     | 53:BU:62:ILE:N     | 2.40                     | 0.55              |
| 54:BV:32:THR:OG1   | 54:BV:60:GLU:HG3   | 2.07                     | 0.55              |
| 57:BY:13:VAL:HG22  | 57:BY:14:LEU:H     | 1.71                     | 0.55              |
| 58:BZ:179:ASP:O    | 58:BZ:180:VAL:C    | 2.44                     | 0.55              |
| 1:CA:474:G:H2'     | 1:CA:475:G:C8      | 2.40                     | 0.55              |
| 1:CA:693:G:C6      | 23:CX:13:A:H1'     | 2.42                     | 0.55              |
| 1:CA:961:U:O2      | 1:CA:983:A:H2'     | 2.06                     | 0.55              |
| 1:CA:1152:A:H5''   | 10:CJ:13:HIS:HD2   | 1.72                     | 0.55              |
| 11:CK:105:VAL:HG23 | 11:CK:105:VAL:O    | 2.06                     | 0.55              |
| 12:CL:76:ASN:O     | 12:CL:76:ASN:CG    | 2.44                     | 0.55              |
| 16:CP:75:ARG:O     | 16:CP:78:GLY:N     | 2.39                     | 0.55              |
| 24:CY:15:ILE:C     | 24:CY:15:ILE:HD12  | 2.27                     | 0.55              |
| 26:D1:86:SER:HA    | 26:D1:89:GLU:CD    | 2.27                     | 0.55              |
| 33:D8:8:LYS:HE3    | 35:DA:245:G:O6     | 2.07                     | 0.55              |
| 35:DA:1907:G:O2'   | 35:DA:1908:C:H5'   | 2.06                     | 0.55              |
| 35:DA:2543:G:N3    | 35:DA:2765:A:H2'   | 2.22                     | 0.55              |
| 35:DA:271(B):C:O2' | 35:DA:271(C):C:H5' | 2.07                     | 0.55              |
| 35:DA:271(F):C:O2' | 35:DA:271(G):C:H5' | 2.05                     | 0.55              |
| 36:DB:103:G:H5''   | 36:DB:104:U:OP2    | 2.05                     | 0.55              |
| 36:DB:114:C:H2'    | 36:DB:115:G:C8     | 2.42                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:DC:190:ILE:O    | 37:DC:194:ILE:HG12 | 2.07                     | 0.55              |
| 41:DG:111:LEU:HB3  | 41:DG:117:PHE:CE2  | 2.41                     | 0.55              |
| 42:DH:68:THR:O     | 42:DH:72:ILE:HG12  | 2.06                     | 0.55              |
| 35:DA:389:G:N1     | 48:DP:71:VAL:HG12  | 2.21                     | 0.55              |
| 52:DT:29:ARG:HG2   | 52:DT:85:LYS:CA    | 2.37                     | 0.55              |
| 54:DV:61:VAL:HG22  | 54:DV:63:GLY:H     | 1.72                     | 0.55              |
| 56:DX:10:ALA:HB1   | 56:DX:11:PRO:HD2   | 1.89                     | 0.55              |
| 1:AA:1141:C:H2'    | 1:AA:1142:G:C8     | 2.42                     | 0.55              |
| 1:AA:1248:A:H2'    | 1:AA:1249:C:H5'    | 1.89                     | 0.55              |
| 1:AA:300:A:H2'     | 1:AA:301:G:O4'     | 2.07                     | 0.55              |
| 2:AB:31:TYR:O      | 2:AB:42:ILE:HG13   | 2.07                     | 0.55              |
| 8:AH:103:VAL:HG12  | 8:AH:108:GLY:HA3   | 1.89                     | 0.55              |
| 10:AJ:78:ASN:O     | 10:AJ:82:ILE:HG12  | 2.06                     | 0.55              |
| 10:AJ:92:THR:HG23  | 10:AJ:93:GLY:N     | 2.22                     | 0.55              |
| 22:AW:41:C:O2'     | 22:AW:42:C:H5'     | 2.07                     | 0.55              |
| 29:B4:53:GLU:OE1   | 29:B4:55:ARG:HD3   | 2.06                     | 0.55              |
| 35:BA:1047:G:N2    | 35:BA:1110:G:H1'   | 2.21                     | 0.55              |
| 35:BA:1274:A:N3    | 35:BA:1297:C:H1'   | 2.21                     | 0.55              |
| 35:BA:1316:U:O2'   | 35:BA:1317:A:H5'   | 2.06                     | 0.55              |
| 35:BA:1336:A:P     | 56:BX:64:LYS:HE3   | 2.46                     | 0.55              |
| 35:BA:1506:C:O2    | 35:BA:1506:C:H2'   | 2.06                     | 0.55              |
| 35:BA:1515:G:H2'   | 35:BA:1516:C:C6    | 2.42                     | 0.55              |
| 35:BA:1759:A:H5'   | 35:BA:2715:C:H1'   | 1.89                     | 0.55              |
| 35:BA:1858:G:H2'   | 35:BA:1883:G:H22   | 1.71                     | 0.55              |
| 35:BA:2132:U:C5    | 37:BC:6:LYS:HD2    | 2.41                     | 0.55              |
| 35:BA:221:A:H4'    | 35:BA:222:A:O5'    | 2.07                     | 0.55              |
| 35:BA:2512:C:H2'   | 35:BA:2513:G:O4'   | 2.07                     | 0.55              |
| 35:BA:271(B):C:O2' | 35:BA:271(C):C:H5' | 2.07                     | 0.55              |
| 35:BA:768:G:H2'    | 35:BA:769:G:H8     | 1.72                     | 0.55              |
| 35:BA:811:U:O2'    | 35:BA:812:C:H5''   | 2.05                     | 0.55              |
| 35:BA:845:G:H8     | 35:BA:845:G:OP2    | 1.89                     | 0.55              |
| 37:BC:149:ASN:HD21 | 37:BC:153:ILE:HD11 | 1.72                     | 0.55              |
| 41:BG:144:ILE:HD11 | 41:BG:149:VAL:HB   | 1.89                     | 0.55              |
| 41:BG:165:THR:O    | 41:BG:167:GLU:N    | 2.40                     | 0.55              |
| 50:BR:7:GLY:O      | 50:BR:8:ARG:CB     | 2.54                     | 0.55              |
| 58:BZ:56:VAL:HG12  | 58:BZ:57:ILE:N     | 2.22                     | 0.55              |
| 1:CA:1166:G:H5'    | 1:CA:1168:A:OP2    | 2.07                     | 0.55              |
| 1:CA:179:A:H2'     | 1:CA:180:U:H6      | 1.68                     | 0.55              |
| 1:CA:509:A:C2      | 1:CA:510:A:C2      | 2.95                     | 0.55              |
| 1:CA:54:C:H2'      | 1:CA:352:C:N4      | 2.21                     | 0.55              |
| 1:CA:658:G:H2'     | 1:CA:659:U:C6      | 2.42                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:796:C:O2      | 1:CA:796:C:H2'     | 2.07                     | 0.55              |
| 2:CB:223:ILE:HG12  | 2:CB:226:ARG:NH1   | 2.22                     | 0.55              |
| 18:CR:85:LEU:HD12  | 18:CR:86:VAL:H     | 1.72                     | 0.55              |
| 1:CA:1318:A:O3'    | 19:CS:10:PHE:CD2   | 2.60                     | 0.55              |
| 20:CT:49:ALA:CB    | 20:CT:99:LEU:HG    | 2.36                     | 0.55              |
| 22:CV:1:C:H2'      | 22:CV:2:G:C8       | 2.42                     | 0.55              |
| 24:CY:111:SER:O    | 24:CY:113:GLY:N    | 2.39                     | 0.55              |
| 24:CY:427:ALA:HB1  | 24:CY:466:LEU:HD11 | 1.88                     | 0.55              |
| 24:CY:491:VAL:HG21 | 24:CY:597:GLY:HA2  | 1.87                     | 0.55              |
| 29:D4:9:LEU:HD13   | 29:D4:26:SER:O     | 2.07                     | 0.55              |
| 19:CS:65:ASN:HA    | 29:D4:48:ARG:NH2   | 2.21                     | 0.55              |
| 35:DA:1141:U:H5''  | 46:DN:63:THR:CG2   | 2.36                     | 0.55              |
| 35:DA:1668:A:N6    | 35:DA:1676:A:H61   | 2.05                     | 0.55              |
| 35:DA:1809:A:H2'   | 35:DA:1810:A:C8    | 2.41                     | 0.55              |
| 35:DA:2532:G:H2'   | 35:DA:2533:A:O4'   | 2.07                     | 0.55              |
| 35:DA:2552:U:O2    | 35:DA:2554:U:H5'   | 2.07                     | 0.55              |
| 35:DA:2733:A:O2'   | 35:DA:2734:A:H5'   | 2.07                     | 0.55              |
| 35:DA:752:A:O2'    | 35:DA:753:C:OP2    | 2.21                     | 0.55              |
| 36:DB:68:C:H2'     | 36:DB:69:G:O4'     | 2.07                     | 0.55              |
| 37:DC:213:VAL:CG1  | 37:DC:225:ILE:HD11 | 2.37                     | 0.55              |
| 39:DE:111:ARG:CZ   | 50:DR:2:ARG:HH21   | 2.20                     | 0.55              |
| 40:DF:10:PRO:HG2   | 40:DF:13:SER:OG    | 2.06                     | 0.55              |
| 40:DF:25:PRO:HG3   | 40:DF:119:ARG:CB   | 2.36                     | 0.55              |
| 40:DF:140:LEU:O    | 40:DF:143:ALA:HB3  | 2.06                     | 0.55              |
| 40:DF:161:GLU:O    | 40:DF:165:ARG:HG3  | 2.06                     | 0.55              |
| 40:DF:8:GLN:NE2    | 40:DF:9:ILE:HB     | 2.21                     | 0.55              |
| 41:DG:37:VAL:HG22  | 41:DG:159:VAL:HA   | 1.88                     | 0.55              |
| 42:DH:157:TYR:CE1  | 42:DH:171:LEU:HD21 | 2.24                     | 0.55              |
| 46:DN:46:VAL:CG1   | 46:DN:47:ALA:H     | 2.13                     | 0.55              |
| 48:DP:107:LYS:HG3  | 48:DP:107:LYS:O    | 2.07                     | 0.55              |
| 51:DS:106:ARG:HD2  | 51:DS:106:ARG:C    | 2.26                     | 0.55              |
| 56:DX:8:ILE:H      | 56:DX:8:ILE:CD1    | 2.17                     | 0.55              |
| 57:DY:86:ARG:HB3   | 57:DY:88:LYS:NZ    | 2.21                     | 0.55              |
| 1:AA:1391:U:H2'    | 1:AA:1392:G:C8     | 2.41                     | 0.55              |
| 1:AA:38:G:C2       | 1:AA:397:A:C2      | 2.94                     | 0.55              |
| 1:AA:628:G:O2'     | 1:AA:629:G:H5'     | 2.07                     | 0.55              |
| 2:AB:33:TYR:HB2    | 2:AB:43:ASP:HB2    | 1.88                     | 0.55              |
| 3:AC:62:ASP:O      | 3:AC:64:VAL:HG23   | 2.07                     | 0.55              |
| 19:AS:33:THR:HG22  | 19:AS:49:ILE:HG22  | 1.87                     | 0.55              |
| 19:AS:72:GLY:O     | 19:AS:74:PHE:N     | 2.40                     | 0.55              |
| 24:AY:105:ILE:HD12 | 24:AY:105:ILE:N    | 2.21                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:AY:156:ARG:HB2  | 24:AY:157:LEU:HD23 | 1.88                     | 0.55              |
| 24:AY:18:ALA:HA    | 24:AY:85:PRO:HG2   | 1.88                     | 0.55              |
| 24:AY:35:TYR:HE1   | 24:AY:269:VAL:HB   | 1.70                     | 0.55              |
| 26:B1:80:LEU:HB3   | 26:B1:82:LEU:HD11  | 1.88                     | 0.55              |
| 31:B6:16:CYS:SG    | 31:B6:48:VAL:CG2   | 2.95                     | 0.55              |
| 34:B9:19:ARG:HB2   | 35:BA:2756:U:H5'   | 1.89                     | 0.55              |
| 35:BA:1044:G:O2'   | 35:BA:1045:A:H5''  | 2.07                     | 0.55              |
| 35:BA:1212:G:O2'   | 35:BA:1236:G:N2    | 2.39                     | 0.55              |
| 35:BA:1301:A:H2'   | 35:BA:1302:A:H3'   | 1.88                     | 0.55              |
| 35:BA:1437:C:H2'   | 35:BA:1438:U:C6    | 2.42                     | 0.55              |
| 35:BA:2792:G:N3    | 35:BA:2792:G:H2'   | 2.22                     | 0.55              |
| 35:BA:27:G:HO2'    | 35:BA:28:A:H8      | 1.52                     | 0.55              |
| 35:BA:612:C:H2'    | 35:BA:613:G:C5'    | 2.15                     | 0.55              |
| 38:BD:166:GLN:HA   | 38:BD:166:GLN:NE2  | 2.21                     | 0.55              |
| 35:BA:2051:A:H4'   | 39:BE:141:ILE:CD1  | 2.37                     | 0.55              |
| 40:BF:206:ILE:HG22 | 40:BF:207:GLY:N    | 2.21                     | 0.55              |
| 46:BN:30:ILE:HG22  | 46:BN:34:LEU:CD2   | 2.37                     | 0.55              |
| 47:BO:9:GLU:HA     | 47:BO:9:GLU:OE1    | 2.06                     | 0.55              |
| 49:BQ:53:ALA:HA    | 49:BQ:56:ARG:HB2   | 1.89                     | 0.55              |
| 52:BT:60:THR:HG22  | 52:BT:77:PRO:HA    | 1.89                     | 0.55              |
| 56:BX:61:GLY:HA3   | 56:BX:73:ARG:O     | 2.07                     | 0.55              |
| 58:BZ:80:ARG:O     | 58:BZ:81:ARG:O     | 2.25                     | 0.55              |
| 1:CA:1030(C):G:H2' | 1:CA:1030(D):A:H8  | 1.71                     | 0.55              |
| 1:CA:1116:C:H2'    | 1:CA:1117:G:C5'    | 2.36                     | 0.55              |
| 1:CA:1141:C:H2'    | 1:CA:1142:G:C8     | 2.42                     | 0.55              |
| 1:CA:1248:A:H2'    | 1:CA:1249:C:H5'    | 1.88                     | 0.55              |
| 1:CA:1351:U:O4'    | 7:CG:33:ASP:HB3    | 2.07                     | 0.55              |
| 1:CA:188:C:H2'     | 1:CA:189:G:C8      | 2.42                     | 0.55              |
| 4:CD:26:CYS:O      | 4:CD:31:CYS:HB2    | 2.07                     | 0.55              |
| 5:CE:12:LEU:HD13   | 5:CE:12:LEU:C      | 2.26                     | 0.55              |
| 12:CL:39:VAL:HB    | 12:CL:57:LYS:HB2   | 1.89                     | 0.55              |
| 13:CM:10:PRO:CG    | 13:CM:18:ALA:HB1   | 2.37                     | 0.55              |
| 13:CM:70:LEU:C     | 13:CM:70:LEU:HD23  | 2.27                     | 0.55              |
| 19:CS:44:MET:HB3   | 19:CS:47:HIS:HD2   | 1.72                     | 0.55              |
| 26:D1:61:ARG:NH1   | 26:D1:61:ARG:HB3   | 2.22                     | 0.55              |
| 35:DA:82:G:C5'     | 35:DA:296:C:H5'    | 2.34                     | 0.55              |
| 38:DD:35:LYS:HG2   | 38:DD:63:ARG:HG3   | 1.89                     | 0.55              |
| 39:DE:119:ARG:HG2  | 39:DE:160:TYR:HB2  | 1.88                     | 0.55              |
| 39:DE:70:ALA:O     | 39:DE:71:GLY:C     | 2.46                     | 0.55              |
| 42:DH:124:GLU:CG   | 42:DH:132:ARG:HG3  | 2.37                     | 0.55              |
| 42:DH:41:MET:O     | 42:DH:42:ARG:CB    | 2.54                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:DH:68:THR:O     | 42:DH:70:THR:N     | 2.40                     | 0.55              |
| 51:DS:36:TYR:N     | 51:DS:36:TYR:CD1   | 2.75                     | 0.55              |
| 52:DT:99:LEU:HB2   | 52:DT:101:PHE:CE1  | 2.42                     | 0.55              |
| 55:DW:1:MET:CE     | 55:DW:2:GLU:H      | 2.20                     | 0.55              |
| 56:DX:12:VAL:O     | 56:DX:13:LEU:HB2   | 2.07                     | 0.55              |
| 1:AA:1300:G:O2'    | 1:AA:1301:U:P      | 2.64                     | 0.55              |
| 1:AA:1329:A:O2'    | 1:AA:1330:U:H5'    | 2.07                     | 0.55              |
| 1:AA:820:U:H4'     | 1:AA:821:G:OP2     | 2.07                     | 0.55              |
| 1:AA:945:G:C2      | 1:AA:946:A:C8      | 2.94                     | 0.55              |
| 2:AB:223:ILE:HG12  | 2:AB:226:ARG:NH1   | 2.22                     | 0.55              |
| 3:AC:101:LEU:C     | 3:AC:101:LEU:HD23  | 2.28                     | 0.55              |
| 3:AC:52:LEU:HD23   | 3:AC:52:LEU:N      | 2.10                     | 0.55              |
| 4:AD:126:ILE:CG2   | 4:AD:127:THR:N     | 2.70                     | 0.55              |
| 6:AF:71:ARG:NH1    | 6:AF:71:ARG:HG3    | 2.20                     | 0.55              |
| 6:AF:4:TYR:HE1     | 6:AF:92:LYS:HD2    | 1.71                     | 0.55              |
| 16:AP:50:LYS:HG2   | 16:AP:51:VAL:H     | 1.71                     | 0.55              |
| 18:AR:74:ARG:HD3   | 18:AR:81:PHE:HD2   | 1.71                     | 0.55              |
| 24:AY:326:THR:O    | 24:AY:328:ILE:HG23 | 2.07                     | 0.55              |
| 24:AY:550:MET:CE   | 24:AY:563:ILE:HD11 | 2.37                     | 0.55              |
| 24:AY:22:ASP:O     | 62:AY:703:GDP:H5'  | 2.07                     | 0.55              |
| 24:AY:86:GLY:O     | 24:AY:88:VAL:N     | 2.37                     | 0.55              |
| 35:BA:1092:C:H2'   | 35:BA:1093:G:H8    | 1.72                     | 0.55              |
| 35:BA:1102:C:H2'   | 35:BA:1103:A:H8    | 1.72                     | 0.55              |
| 35:BA:1205:U:C5    | 40:BF:171:PRO:HA   | 2.42                     | 0.55              |
| 35:BA:1600:C:O2'   | 35:BA:1601:G:H5'   | 2.07                     | 0.55              |
| 35:BA:1332:G:N2    | 35:BA:1609:A:H3'   | 2.22                     | 0.55              |
| 35:BA:15:G:O2'     | 35:BA:16:G:H5'     | 2.06                     | 0.55              |
| 35:BA:2336:A:N3    | 35:BA:2385:C:H1'   | 2.22                     | 0.55              |
| 40:BF:161:GLU:O    | 40:BF:165:ARG:HG3  | 2.06                     | 0.55              |
| 46:BN:15:LEU:HD13  | 46:BN:16:ILE:N     | 2.21                     | 0.55              |
| 48:BP:146:VAL:HG22 | 48:BP:147:LEU:N    | 2.12                     | 0.55              |
| 48:BP:30:THR:O     | 48:BP:33:ARG:N     | 2.27                     | 0.55              |
| 52:BT:10:VAL:C     | 52:BT:12:SER:N     | 2.57                     | 0.55              |
| 53:BU:106:PHE:O    | 53:BU:109:LEU:N    | 2.40                     | 0.55              |
| 57:BY:67:LEU:HD11  | 57:BY:71:LYS:HE2   | 1.87                     | 0.55              |
| 1:CA:1346:A:N6     | 1:CA:1374:A:H3'    | 2.21                     | 0.55              |
| 1:CA:1431:C:C2'    | 1:CA:1432:G:H5'    | 2.37                     | 0.55              |
| 1:CA:241:C:O2'     | 1:CA:242:C:H5'     | 2.07                     | 0.55              |
| 2:CB:54:THR:HG22   | 2:CB:58:ILE:HD11   | 1.89                     | 0.55              |
| 6:CF:91:VAL:HG12   | 6:CF:92:LYS:N      | 2.21                     | 0.55              |
| 10:CJ:3:LYS:NZ     | 10:CJ:76:ASN:HA    | 2.20                     | 0.55              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:CM:6:GLY:O      | 13:CM:8:GLU:N      | 2.40                     | 0.55              |
| 24:CY:142:THR:C    | 24:CY:144:ALA:H    | 2.10                     | 0.55              |
| 24:CY:309:LEU:O    | 24:CY:390:VAL:HG12 | 2.07                     | 0.55              |
| 1:CA:395:C:O3'     | 24:CY:349:LYS:NZ   | 2.39                     | 0.55              |
| 24:CY:96:ARG:HG3   | 24:CY:403:GLU:OE2  | 2.07                     | 0.55              |
| 31:D6:7:ILE:O      | 31:D6:27:LYS:HD3   | 2.07                     | 0.55              |
| 31:D6:27:LYS:HZ2   | 31:D6:30:THR:HB    | 1.70                     | 0.55              |
| 35:DA:1047:G:N2    | 35:DA:1110:G:H1'   | 2.21                     | 0.55              |
| 35:DA:2746:U:O2'   | 35:DA:2747:G:H5'   | 2.06                     | 0.55              |
| 35:DA:2818:G:O2'   | 35:DA:2837:G:H5'   | 2.07                     | 0.55              |
| 35:DA:438:G:O2'    | 35:DA:440:G:H5'    | 2.07                     | 0.55              |
| 35:DA:58:G:H1      | 35:DA:69:C:H42     | 1.53                     | 0.55              |
| 35:DA:654(L):G:H2' | 35:DA:654(M):C:H4' | 1.88                     | 0.55              |
| 35:DA:2679:A:H4'   | 39:DE:165:VAL:HG11 | 1.89                     | 0.55              |
| 41:DG:10:LYS:HE3   | 41:DG:14:GLU:OE2   | 2.06                     | 0.55              |
| 41:DG:60:LEU:HD22  | 41:DG:63:ILE:CD1   | 2.36                     | 0.55              |
| 42:DH:127:GLU:HB3  | 42:DH:128:PRO:HD2  | 1.89                     | 0.55              |
| 46:DN:15:LEU:HD13  | 46:DN:16:ILE:N     | 2.22                     | 0.55              |
| 46:DN:3:THR:C      | 46:DN:4:TYR:CG     | 2.80                     | 0.55              |
| 47:DO:52:VAL:O     | 47:DO:53:LYS:HG3   | 2.07                     | 0.55              |
| 48:DP:108:LYS:HD2  | 48:DP:108:LYS:N    | 2.22                     | 0.55              |
| 48:DP:127:ALA:HB3  | 48:DP:130:PHE:CZ   | 2.42                     | 0.55              |
| 48:DP:127:ALA:O    | 48:DP:148:LEU:HD11 | 2.06                     | 0.55              |
| 50:DR:45:ARG:CG    | 50:DR:46:GLY:H     | 2.15                     | 0.55              |
| 52:DT:27:THR:OG1   | 52:DT:28:VAL:N     | 2.39                     | 0.55              |
| 1:AA:1082:G:O2'    | 1:AA:1083:U:H5'    | 2.07                     | 0.54              |
| 1:AA:1101:A:H4'    | 1:AA:1102:A:C4'    | 2.37                     | 0.54              |
| 3:AC:133:ALA:O     | 3:AC:137:ALA:HB2   | 2.06                     | 0.54              |
| 5:AE:76:ILE:CG2    | 5:AE:118:ILE:HD13  | 2.37                     | 0.54              |
| 6:AF:37:VAL:HG12   | 6:AF:38:GLU:O      | 2.07                     | 0.54              |
| 6:AF:10:LEU:HD12   | 6:AF:61:LEU:HD13   | 1.88                     | 0.54              |
| 5:AE:143:ARG:HH12  | 8:AH:77:GLU:CD     | 2.10                     | 0.54              |
| 12:AL:60:LEU:HD22  | 12:AL:60:LEU:N     | 2.22                     | 0.54              |
| 13:AM:49:THR:O     | 13:AM:53:VAL:HG23  | 2.07                     | 0.54              |
| 19:AS:13:ASP:O     | 19:AS:15:LEU:N     | 2.40                     | 0.54              |
| 20:AT:13:LEU:O     | 20:AT:16:HIS:N     | 2.40                     | 0.54              |
| 24:AY:121:VAL:HA   | 24:AY:124:GLN:HE22 | 1.72                     | 0.54              |
| 35:BA:1245:G:C5'   | 40:BF:34:TRP:HZ2   | 2.20                     | 0.54              |
| 35:BA:1358:G:O2'   | 35:BA:1359:A:H5''  | 2.08                     | 0.54              |
| 35:BA:1556:C:H2'   | 35:BA:1557:C:C6    | 2.42                     | 0.54              |
| 35:BA:961:C:N4     | 35:BA:2031:A:H1'   | 2.22                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:BA:208:C:H2'    | 35:BA:209:C:H6    | 1.72                     | 0.54              |
| 35:BA:2230:G:H2'   | 35:BA:2231:C:H6   | 1.72                     | 0.54              |
| 35:BA:272(H):C:C5' | 35:BA:272(H):C:H6 | 2.18                     | 0.54              |
| 35:BA:359:A:H2'    | 35:BA:360:G:O4'   | 2.07                     | 0.54              |
| 35:BA:74:A:O2'     | 35:BA:75:G:OP2    | 2.23                     | 0.54              |
| 36:BB:16:G:N2      | 36:BB:69:G:H1'    | 2.22                     | 0.54              |
| 36:BB:77:U:O2'     | 36:BB:78:A:H5'    | 2.07                     | 0.54              |
| 37:BC:11:LEU:O     | 37:BC:13:GLU:N    | 2.40                     | 0.54              |
| 35:BA:2820:A:C8    | 39:BE:191:PRO:HB2 | 2.42                     | 0.54              |
| 50:BR:85:PRO:C     | 50:BR:87:TYR:H    | 2.10                     | 0.54              |
| 52:BT:12:SER:O     | 52:BT:13:ARG:NH2  | 2.40                     | 0.54              |
| 55:BW:1:MET:CE     | 55:BW:2:GLU:H     | 2.19                     | 0.54              |
| 57:BY:96:ILE:CG2   | 57:BY:99:CYS:HB3  | 2.37                     | 0.54              |
| 2:CB:114:ARG:HD2   | 2:CB:118:LEU:HG   | 1.89                     | 0.54              |
| 5:CE:10:MET:HG3    | 5:CE:32:VAL:HG22  | 1.88                     | 0.54              |
| 5:CE:76:ILE:HG13   | 5:CE:77:PRO:HD2   | 1.87                     | 0.54              |
| 12:CL:111:LYS:O    | 12:CL:112:ASP:HB2 | 2.07                     | 0.54              |
| 22:CV:37:A:H3'     | 22:CV:38:A:H8     | 1.71                     | 0.54              |
| 24:CY:539:ILE:HA   | 24:CY:542:VAL:CG1 | 2.37                     | 0.54              |
| 22:CW:76:C:OP1     | 26:D1:30:VAL:HG21 | 2.06                     | 0.54              |
| 26:D1:80:LEU:HD23  | 26:D1:81:LYS:H    | 1.70                     | 0.54              |
| 35:DA:1661:G:O2'   | 35:DA:1662:C:H5'  | 2.07                     | 0.54              |
| 35:DA:1683:C:H2'   | 35:DA:1684:C:C6   | 2.41                     | 0.54              |
| 35:DA:1943:U:O2'   | 35:DA:1944:U:H3'  | 2.07                     | 0.54              |
| 35:DA:1943:U:O2'   | 35:DA:1944:U:O5'  | 2.22                     | 0.54              |
| 35:DA:2008:C:H2'   | 35:DA:2009:G:C8   | 2.42                     | 0.54              |
| 37:DC:14:LYS:O     | 37:DC:15:VAL:HG13 | 2.08                     | 0.54              |
| 38:DD:241:PRO:O    | 38:DD:242:ARG:CB  | 2.55                     | 0.54              |
| 39:DE:28:ALA:HB3   | 39:DE:93:VAL:HG22 | 1.90                     | 0.54              |
| 39:DE:94:GLU:OE2   | 39:DE:177:PRO:HB3 | 2.07                     | 0.54              |
| 43:DJ:72:UNK:C     | 43:DJ:74:UNK:N    | 2.69                     | 0.54              |
| 44:DK:6:ALA:O      | 44:DK:58:THR:HA   | 2.07                     | 0.54              |
| 46:DN:95:PRO:HA    | 46:DN:98:VAL:HG23 | 1.88                     | 0.54              |
| 47:DO:9:GLU:OE1    | 47:DO:9:GLU:HA    | 2.07                     | 0.54              |
| 48:DP:45:LEU:HG    | 48:DP:46:LYS:H    | 1.70                     | 0.54              |
| 25:D0:5:LYS:HB2    | 49:DQ:80:GLU:O    | 2.07                     | 0.54              |
| 54:DV:38:LEU:H     | 54:DV:51:VAL:HG13 | 1.72                     | 0.54              |
| 1:AA:1008:C:H2'    | 1:AA:1009:G:H8    | 1.71                     | 0.54              |
| 1:AA:1366:C:H2'    | 1:AA:1367:C:H6    | 1.73                     | 0.54              |
| 1:AA:961:U:O2      | 1:AA:983:A:H2'    | 2.08                     | 0.54              |
| 1:AA:973:G:H1'     | 10:AJ:55:LYS:HZ3  | 1.71                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:AD:8:VAL:O       | 4:AD:10:ARG:N     | 2.34                     | 0.54              |
| 5:AE:51:VAL:O      | 5:AE:55:VAL:HG23  | 2.07                     | 0.54              |
| 8:AH:103:VAL:HG21  | 8:AH:110:ALA:HB2  | 1.88                     | 0.54              |
| 14:AN:37:PHE:CE1   | 14:AN:53:LEU:HD22 | 2.42                     | 0.54              |
| 16:AP:18:ARG:HD3   | 16:AP:35:LYS:HD2  | 1.88                     | 0.54              |
| 24:AY:228:MET:HE2  | 24:AY:229:LEU:HG  | 1.90                     | 0.54              |
| 24:AY:359:HIS:O    | 24:AY:361:ASN:N   | 2.40                     | 0.54              |
| 24:AY:65:ILE:HD13  | 24:AY:65:ILE:H    | 1.71                     | 0.54              |
| 24:AY:610:VAL:HG12 | 24:AY:669:PHE:HB3 | 1.88                     | 0.54              |
| 27:B2:69:ARG:HH22  | 35:BA:111:A:C5'   | 2.21                     | 0.54              |
| 35:BA:1404:C:O2'   | 35:BA:1405:U:H5'  | 2.07                     | 0.54              |
| 35:BA:1788:C:H2'   | 35:BA:1789:A:H8   | 1.71                     | 0.54              |
| 35:BA:2532:G:H2'   | 35:BA:2533:A:O4'  | 2.07                     | 0.54              |
| 35:BA:322:A:H5'    | 35:BA:340:A:H1'   | 1.89                     | 0.54              |
| 35:BA:548:A:C3'    | 35:BA:549:G:H5'   | 2.38                     | 0.54              |
| 38:BD:61:LEU:HB3   | 38:BD:63:ARG:HH12 | 1.72                     | 0.54              |
| 39:BE:28:ALA:HB3   | 39:BE:93:VAL:HG22 | 1.88                     | 0.54              |
| 41:BG:63:ILE:CA    | 41:BG:143:GLU:HG3 | 2.25                     | 0.54              |
| 43:BJ:52:UNK:O     | 43:BJ:53:UNK:CB   | 2.54                     | 0.54              |
| 46:BN:9:VAL:HG12   | 46:BN:10:GLU:N    | 2.22                     | 0.54              |
| 48:BP:135:LEU:HD13 | 48:BP:135:LEU:O   | 2.06                     | 0.54              |
| 51:BS:70:GLY:C     | 51:BS:72:ALA:H    | 2.10                     | 0.54              |
| 52:BT:27:THR:OG1   | 52:BT:28:VAL:N    | 2.40                     | 0.54              |
| 52:BT:3:ARG:O      | 52:BT:4:GLY:C     | 2.44                     | 0.54              |
| 35:BA:1252:G:N3    | 53:BU:33:ARG:HD2  | 2.21                     | 0.54              |
| 54:BV:1:MET:HA     | 54:BV:1:MET:HE2   | 1.89                     | 0.54              |
| 54:BV:82:ARG:HD2   | 54:BV:82:ARG:N    | 2.23                     | 0.54              |
| 57:BY:44:ILE:HG22  | 57:BY:45:VAL:N    | 2.18                     | 0.54              |
| 58:BZ:63:ASP:OD2   | 58:BZ:65:GLN:NE2  | 2.40                     | 0.54              |
| 58:BZ:71:VAL:HG13  | 58:BZ:86:VAL:CG1  | 2.37                     | 0.54              |
| 1:CA:1347:G:O2'    | 1:CA:1348:U:P     | 2.65                     | 0.54              |
| 2:CB:20:GLU:HB2    | 2:CB:190:THR:OG1  | 2.07                     | 0.54              |
| 3:CC:15:THR:CG2    | 3:CC:181:ASN:HA   | 2.38                     | 0.54              |
| 4:CD:150:GLU:HG2   | 4:CD:151:LYS:N    | 2.22                     | 0.54              |
| 9:CI:40:LEU:CD1    | 9:CI:70:LYS:HG2   | 2.35                     | 0.54              |
| 15:CO:76:GLU:O     | 15:CO:78:TYR:N    | 2.39                     | 0.54              |
| 24:CY:282:SER:O    | 24:CY:284:LEU:N   | 2.40                     | 0.54              |
| 24:CY:603:GLU:OE1  | 24:CY:648:PRO:HB3 | 2.07                     | 0.54              |
| 26:D1:82:LEU:C     | 26:D1:83:GLU:HG3  | 2.28                     | 0.54              |
| 34:D9:10:ILE:O     | 34:D9:11:CYS:HB3  | 2.06                     | 0.54              |
| 35:DA:110:G:O2'    | 35:DA:111:A:H5'   | 2.08                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 35:DA:1287:A:H2'   | 35:DA:1287:A:N3     | 2.20                     | 0.54              |
| 35:DA:1336:A:OP2   | 56:DX:64:LYS:HE3    | 2.08                     | 0.54              |
| 35:DA:135:G:O2'    | 35:DA:136:G:H5'     | 2.07                     | 0.54              |
| 35:DA:2067:G:H1    | 35:DA:2443:C:H42    | 1.55                     | 0.54              |
| 35:DA:271(K):U:H3' | 35:DA:271(L):U:H5'' | 1.88                     | 0.54              |
| 35:DA:2839:G:H2'   | 35:DA:2840:C:C6     | 2.42                     | 0.54              |
| 35:DA:426:C:O2'    | 35:DA:427:U:H5'     | 2.06                     | 0.54              |
| 35:DA:848:G:C2     | 35:DA:933:A:H1'     | 2.41                     | 0.54              |
| 38:DD:26:LYS:H     | 38:DD:26:LYS:HE2    | 1.72                     | 0.54              |
| 42:DH:86:GLU:HB3   | 42:DH:132:ARG:HB3   | 1.88                     | 0.54              |
| 42:DH:20:ALA:HB1   | 42:DH:21:PRO:HD2    | 1.89                     | 0.54              |
| 43:DJ:146:UNK:C    | 43:DJ:148:UNK:N     | 2.69                     | 0.54              |
| 44:DK:112:MET:HE2  | 44:DK:120:LEU:HD21  | 1.89                     | 0.54              |
| 35:DA:751:A:C5'    | 55:DW:90:ARG:HA     | 2.36                     | 0.54              |
| 27:D2:29:LYS:HZ2   | 56:DX:3:THR:N       | 2.06                     | 0.54              |
| 1:AA:1005:A:H5'    | 1:AA:1006:C:OP2     | 2.07                     | 0.54              |
| 1:AA:1208:C:H2'    | 1:AA:1209:C:H6      | 1.72                     | 0.54              |
| 1:AA:1325:C:H2'    | 1:AA:1326:C:C6      | 2.42                     | 0.54              |
| 1:AA:264:U:H4'     | 17:AQ:63:ARG:HD3    | 1.89                     | 0.54              |
| 1:AA:715:A:H2'     | 1:AA:716:A:H8       | 1.71                     | 0.54              |
| 1:AA:93:G:O2'      | 1:AA:96:U:H5'       | 2.06                     | 0.54              |
| 3:AC:46:GLU:O      | 3:AC:47:LEU:CB      | 2.54                     | 0.54              |
| 5:AE:135:THR:O     | 5:AE:138:ALA:HB3    | 2.06                     | 0.54              |
| 6:AF:47:ARG:HH11   | 6:AF:47:ARG:HG2     | 1.73                     | 0.54              |
| 7:AG:140:ASP:O     | 7:AG:144:MET:HG2    | 2.07                     | 0.54              |
| 13:AM:77:ASN:O     | 13:AM:80:ARG:N      | 2.36                     | 0.54              |
| 24:AY:286:ILE:N    | 24:AY:286:ILE:HD12  | 2.23                     | 0.54              |
| 25:B0:51:VAL:HG21  | 25:B0:79:VAL:O      | 2.08                     | 0.54              |
| 26:B1:29:GLY:C     | 26:B1:31:GLY:N      | 2.61                     | 0.54              |
| 26:B1:85:LEU:O     | 26:B1:87:PRO:HD2    | 2.08                     | 0.54              |
| 33:B8:32:LEU:HB3   | 33:B8:36:LYS:NZ     | 2.22                     | 0.54              |
| 35:BA:110:G:O2'    | 35:BA:111:A:H5'     | 2.06                     | 0.54              |
| 35:BA:1902:C:H2'   | 35:BA:1903:G:O4'    | 2.06                     | 0.54              |
| 35:BA:2245:U:C5'   | 35:BA:2246:G:H5'    | 2.33                     | 0.54              |
| 35:BA:260:G:H1'    | 35:BA:621:A:H1'     | 1.89                     | 0.54              |
| 35:BA:936:C:H2'    | 35:BA:937:U:H6      | 1.70                     | 0.54              |
| 37:BC:139:PRO:HA   | 37:BC:145:THR:CG2   | 2.37                     | 0.54              |
| 37:BC:190:ILE:O    | 37:BC:194:ILE:HG12  | 2.06                     | 0.54              |
| 40:BF:24:LEU:HB3   | 40:BF:25:PRO:CD     | 2.32                     | 0.54              |
| 42:BH:148:ILE:O    | 42:BH:151:ILE:HG12  | 2.07                     | 0.54              |
| 44:BK:29:GLN:O     | 44:BK:59:ILE:HD12   | 2.07                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:BN:109:LYS:H   | 46:BN:109:LYS:CE   | 2.21                     | 0.54              |
| 46:BN:65:LYS:NZ   | 46:BN:65:LYS:HA    | 2.22                     | 0.54              |
| 48:BP:107:LYS:C   | 48:BP:109:GLY:H    | 2.09                     | 0.54              |
| 48:BP:38:GLN:HG3  | 48:BP:39:LYS:N     | 2.12                     | 0.54              |
| 51:BS:51:ALA:HB3  | 51:BS:73:LEU:HD12  | 1.89                     | 0.54              |
| 52:BT:106:SER:O   | 52:BT:107:ASP:CB   | 2.55                     | 0.54              |
| 52:BT:10:VAL:O    | 52:BT:13:ARG:HG2   | 2.06                     | 0.54              |
| 57:BY:91:GLU:O    | 57:BY:92:ASN:HB2   | 2.07                     | 0.54              |
| 1:CA:1060:C:H5'   | 14:CN:45:ARG:NH2   | 2.23                     | 0.54              |
| 1:CA:1149:C:H2'   | 1:CA:1150:U:C6     | 2.42                     | 0.54              |
| 1:CA:1198:G:H2'   | 1:CA:1199:U:O4'    | 2.06                     | 0.54              |
| 1:CA:1316:G:N2    | 1:CA:1318:A:H3'    | 2.22                     | 0.54              |
| 1:CA:663:A:O2'    | 1:CA:664:G:H5'     | 2.07                     | 0.54              |
| 1:CA:665:A:H2'    | 1:CA:732:C:O2      | 2.07                     | 0.54              |
| 2:CB:44:LEU:HA    | 2:CB:47:THR:OG1    | 2.07                     | 0.54              |
| 4:CD:153:ARG:HG2  | 4:CD:153:ARG:HH11  | 1.73                     | 0.54              |
| 8:CH:103:VAL:HG23 | 8:CH:110:ALA:HB2   | 1.89                     | 0.54              |
| 8:CH:119:LEU:HD12 | 8:CH:124:ALA:HB2   | 1.88                     | 0.54              |
| 9:CI:4:TYR:CE2    | 9:CI:59:PHE:HE2    | 2.26                     | 0.54              |
| 17:CQ:99:SER:C    | 17:CQ:100:LYS:HG3  | 2.27                     | 0.54              |
| 24:CY:16:GLY:O    | 24:CY:104:ALA:CB   | 2.54                     | 0.54              |
| 24:CY:507:TYR:CD1 | 24:CY:507:TYR:C    | 2.80                     | 0.54              |
| 25:D0:40:GLN:HE22 | 25:D0:43:THR:CA    | 2.19                     | 0.54              |
| 26:D1:11:ARG:NH2  | 35:DA:1365:A:O2'   | 2.40                     | 0.54              |
| 29:D4:12:ALA:HB1  | 29:D4:29:PRO:HA    | 1.89                     | 0.54              |
| 30:D5:4:HIS:HB3   | 30:D5:5:PRO:CD     | 2.32                     | 0.54              |
| 30:D5:56:LYS:CG   | 30:D5:57:VAL:H     | 2.05                     | 0.54              |
| 35:DA:1301:A:H2'  | 35:DA:1302:A:H3'   | 1.88                     | 0.54              |
| 35:DA:2657:A:H2'  | 35:DA:2658:C:C5'   | 2.35                     | 0.54              |
| 35:DA:2777:G:H5'' | 35:DA:2778:A:H5''  | 1.88                     | 0.54              |
| 35:DA:28:A:H62    | 35:DA:512:G:H1'    | 1.72                     | 0.54              |
| 35:DA:993:G:OP1   | 53:DU:50:ARG:HD2   | 2.07                     | 0.54              |
| 36:DB:7:G:H5'     | 51:DS:29:PHE:CD1   | 2.41                     | 0.54              |
| 39:DE:55:ASN:O    | 39:DE:57:LYS:N     | 2.33                     | 0.54              |
| 41:DG:57:ALA:O    | 41:DG:68:PRO:HG2   | 2.07                     | 0.54              |
| 44:DK:78:ILE:HD13 | 44:DK:134:MET:SD   | 2.47                     | 0.54              |
| 48:DP:100:LEU:HA  | 48:DP:103:ALA:HB3  | 1.87                     | 0.54              |
| 48:DP:83:VAL:H    | 48:DP:115:LEU:HD21 | 1.72                     | 0.54              |
| 35:DA:941:A:H4'   | 48:DP:35:HIS:CE1   | 2.42                     | 0.54              |
| 49:DQ:35:VAL:HG22 | 49:DQ:36:ALA:N     | 2.22                     | 0.54              |
| 51:DS:98:VAL:CG1  | 51:DS:100:ALA:HB2  | 2.38                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 54:DV:37:VAL:HG23  | 54:DV:37:VAL:O     | 2.07                     | 0.54              |
| 56:DX:18:TYR:C     | 56:DX:20:GLY:N     | 2.59                     | 0.54              |
| 57:DY:94:LYS:O     | 57:DY:102:CYS:HB2  | 2.06                     | 0.54              |
| 57:DY:15:VAL:O     | 57:DY:22:GLY:N     | 2.40                     | 0.54              |
| 1:AA:953:G:O6      | 1:AA:1228:C:N4     | 2.39                     | 0.54              |
| 1:AA:1378:C:OP1    | 7:AG:7:ALA:HB3     | 2.08                     | 0.54              |
| 1:AA:261:U:H2'     | 1:AA:263:A:OP2     | 2.08                     | 0.54              |
| 1:AA:631:G:H5'     | 1:AA:631:G:H8      | 1.71                     | 0.54              |
| 2:AB:9:GLU:N       | 2:AB:9:GLU:OE2     | 2.40                     | 0.54              |
| 3:AC:128:PHE:O     | 3:AC:130:VAL:N     | 2.40                     | 0.54              |
| 12:AL:41:ARG:NH1   | 12:AL:41:ARG:HB3   | 2.16                     | 0.54              |
| 12:AL:41:ARG:HG2   | 12:AL:42:THR:N     | 2.18                     | 0.54              |
| 17:AQ:59:ILE:HG23  | 17:AQ:71:PHE:CB    | 2.34                     | 0.54              |
| 24:AY:250:THR:HA   | 24:AY:255:ILE:HG23 | 1.89                     | 0.54              |
| 24:AY:137:ASN:HD21 | 24:AY:263:ALA:HB3  | 1.73                     | 0.54              |
| 24:AY:343:ASN:HD21 | 24:AY:345:THR:CB   | 2.20                     | 0.54              |
| 25:B0:20:ARG:CD    | 25:B0:20:ARG:H     | 2.21                     | 0.54              |
| 27:B2:55:ARG:O     | 27:B2:58:ALA:HB3   | 2.07                     | 0.54              |
| 29:B4:19:GLY:O     | 29:B4:21:VAL:HG23  | 2.08                     | 0.54              |
| 31:B6:53:LYS:HG3   | 31:B6:54:ILE:HG23  | 1.89                     | 0.54              |
| 35:BA:1196:C:O2'   | 35:BA:1227:G:H4'   | 2.07                     | 0.54              |
| 35:BA:1344:G:H5'   | 35:BA:1384:A:C6    | 2.42                     | 0.54              |
| 35:BA:1539:G:H2'   | 35:BA:1540:U:O4'   | 2.06                     | 0.54              |
| 35:BA:1658:C:OP1   | 39:BE:132:HIS:O    | 2.26                     | 0.54              |
| 35:BA:2478:A:H2'   | 35:BA:2479:G:O4'   | 2.08                     | 0.54              |
| 35:BA:613:G:H5'    | 35:BA:613:G:C8     | 2.43                     | 0.54              |
| 38:BD:26:LYS:H     | 38:BD:26:LYS:HE2   | 1.72                     | 0.54              |
| 40:BF:39:TRP:CB    | 40:BF:101:LEU:HD22 | 2.37                     | 0.54              |
| 47:BO:113:LYS:O    | 47:BO:117:LEU:HD12 | 2.07                     | 0.54              |
| 57:BY:38:ILE:HG23  | 57:BY:39:VAL:N     | 2.23                     | 0.54              |
| 1:CA:1005:A:H5'    | 1:CA:1006:C:OP2    | 2.07                     | 0.54              |
| 1:CA:1517:G:H1'    | 35:DA:1919:A:O3'   | 2.06                     | 0.54              |
| 1:CA:759:A:H2'     | 1:CA:760:G:H5'     | 1.89                     | 0.54              |
| 3:CC:141:VAL:HG12  | 3:CC:146:ALA:HB3   | 1.89                     | 0.54              |
| 3:CC:46:GLU:HB3    | 3:CC:83:ARG:HH22   | 1.71                     | 0.54              |
| 5:CE:101:ILE:HD11  | 5:CE:119:LEU:HD22  | 1.89                     | 0.54              |
| 11:CK:21:ILE:HG13  | 11:CK:30:VAL:HG12  | 1.89                     | 0.54              |
| 12:CL:119:LYS:O    | 12:CL:120:TYR:HB2  | 2.08                     | 0.54              |
| 15:CO:17:ARG:HG3   | 15:CO:17:ARG:HH11  | 1.72                     | 0.54              |
| 20:CT:48:LYS:HB3   | 20:CT:51:GLU:CG    | 2.37                     | 0.54              |
| 20:CT:73:HIS:O     | 20:CT:74:LYS:C     | 2.46                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:CX:11:U:H4'     | 23:CX:12:A:O5'     | 2.05                     | 0.54              |
| 24:CY:192:LEU:HD12 | 24:CY:194:THR:CG2  | 2.37                     | 0.54              |
| 24:CY:373:ASP:C    | 24:CY:374:LEU:HD12 | 2.28                     | 0.54              |
| 24:CY:609:GLU:CG   | 24:CY:670:VAL:HG21 | 2.38                     | 0.54              |
| 31:D6:15:GLU:C     | 31:D6:16:CYS:O     | 2.45                     | 0.54              |
| 32:D7:24:THR:HG23  | 32:D7:27:GLY:CA    | 2.37                     | 0.54              |
| 35:DA:1040:C:C4    | 35:DA:1041:C:C4    | 2.95                     | 0.54              |
| 35:DA:1225:G:H2'   | 35:DA:1226:A:C8    | 2.43                     | 0.54              |
| 35:DA:1461:G:O2'   | 35:DA:1462:C:H5'   | 2.08                     | 0.54              |
| 35:DA:2000:G:O2'   | 35:DA:2001:A:H5'   | 2.06                     | 0.54              |
| 35:DA:2107:C:H42   | 35:DA:2182:G:H1    | 1.56                     | 0.54              |
| 26:D1:40:ARG:HH12  | 35:DA:2232:U:P     | 2.30                     | 0.54              |
| 35:DA:2733:A:H2'   | 35:DA:2734:A:O4'   | 2.08                     | 0.54              |
| 35:DA:495:G:H1'    | 55:DW:57:ASN:OD1   | 2.07                     | 0.54              |
| 35:DA:651:G:H2'    | 35:DA:652:C:H5'    | 1.88                     | 0.54              |
| 37:DC:11:LEU:O     | 37:DC:13:GLU:N     | 2.41                     | 0.54              |
| 37:DC:149:ASN:HD21 | 37:DC:153:ILE:HD11 | 1.73                     | 0.54              |
| 35:DA:2122:U:H1'   | 37:DC:167:ASP:OD2  | 2.06                     | 0.54              |
| 38:DD:118:VAL:HG22 | 38:DD:119:ALA:N    | 2.22                     | 0.54              |
| 41:DG:59:GLU:OE2   | 41:DG:138:GLN:NE2  | 2.40                     | 0.54              |
| 41:DG:145:THR:HG21 | 41:DG:148:MET:HB2  | 1.89                     | 0.54              |
| 41:DG:147:ASP:C    | 41:DG:149:VAL:H    | 2.11                     | 0.54              |
| 45:DL:15:UNK:C     | 45:DL:17:UNK:N     | 2.66                     | 0.54              |
| 46:DN:109:LYS:H    | 46:DN:109:LYS:CE   | 2.20                     | 0.54              |
| 46:DN:30:ILE:HG22  | 46:DN:34:LEU:CD2   | 2.37                     | 0.54              |
| 46:DN:55:VAL:HG22  | 46:DN:56:ASN:H     | 1.72                     | 0.54              |
| 49:DQ:41:TRP:HE1   | 49:DQ:96:VAL:HG22  | 1.71                     | 0.54              |
| 50:DR:113:LEU:HD12 | 50:DR:114:VAL:H    | 1.72                     | 0.54              |
| 35:DA:1276:A:H1'   | 50:DR:16:HIS:HE1   | 1.73                     | 0.54              |
| 51:DS:51:ALA:HB3   | 51:DS:73:LEU:HB2   | 1.89                     | 0.54              |
| 51:DS:49:VAL:HG21  | 51:DS:77:ALA:HB2   | 1.89                     | 0.54              |
| 1:AA:1053:G:H4'    | 1:AA:1054:C:H5'    | 1.90                     | 0.54              |
| 1:AA:129(A):G:H5'' | 1:AA:129(A):G:C8   | 2.42                     | 0.54              |
| 1:AA:189(K):U:H2'  | 1:AA:189(L):G:C8   | 2.43                     | 0.54              |
| 1:AA:539:A:H2'     | 1:AA:540:G:H8      | 1.72                     | 0.54              |
| 3:AC:167:TRP:O     | 3:AC:168:ALA:HB3   | 2.07                     | 0.54              |
| 4:AD:57:ARG:HG2    | 4:AD:57:ARG:HH11   | 1.72                     | 0.54              |
| 8:AH:119:LEU:HD12  | 8:AH:124:ALA:HB2   | 1.89                     | 0.54              |
| 8:AH:7:ALA:HB2     | 8:AH:85:ARG:HD3    | 1.89                     | 0.54              |
| 1:AA:1148:U:O3'    | 9:AI:14:VAL:HG11   | 2.06                     | 0.54              |
| 9:AI:81:ILE:O      | 9:AI:85:LEU:HG     | 2.08                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:AI:4:TYR:CE2     | 9:AI:88:TYR:CB     | 2.90                     | 0.54              |
| 10:AJ:20:ALA:C     | 10:AJ:22:LYS:N     | 2.61                     | 0.54              |
| 10:AJ:33:GLN:HB2   | 10:AJ:75:ILE:HD13  | 1.89                     | 0.54              |
| 13:AM:6:GLY:O      | 13:AM:8:GLU:N      | 2.39                     | 0.54              |
| 18:AR:85:LEU:HD12  | 18:AR:86:VAL:H     | 1.71                     | 0.54              |
| 19:AS:29:ARG:O     | 19:AS:31:ILE:N     | 2.34                     | 0.54              |
| 24:AY:608:VAL:HG13 | 24:AY:670:VAL:O    | 2.08                     | 0.54              |
| 24:AY:601:ILE:HG21 | 24:AY:687:LEU:HD12 | 1.88                     | 0.54              |
| 24:AY:87:HIS:O     | 24:AY:88:VAL:C     | 2.45                     | 0.54              |
| 28:B3:31:LEU:O     | 28:B3:32:GLN:HB2   | 2.06                     | 0.54              |
| 35:BA:1240:U:O2'   | 35:BA:1241:A:H5'   | 2.08                     | 0.54              |
| 35:BA:1910:G:O2'   | 35:BA:1911:U:H5'   | 2.08                     | 0.54              |
| 35:BA:1947:C:H2'   | 35:BA:1948:G:C5'   | 2.32                     | 0.54              |
| 35:BA:2291:U:H2'   | 35:BA:2292:C:H6    | 1.71                     | 0.54              |
| 35:BA:2299:G:O2'   | 35:BA:2300:G:H5'   | 2.06                     | 0.54              |
| 35:BA:2531:A:OP1   | 42:BH:177:GLY:C    | 2.46                     | 0.54              |
| 35:BA:71:A:H4'     | 35:BA:72:U:H5''    | 1.89                     | 0.54              |
| 35:BA:946:G:H2'    | 35:BA:947:G:C8     | 2.42                     | 0.54              |
| 40:BF:187:VAL:HG12 | 48:BP:7:ARG:NH2    | 2.22                     | 0.54              |
| 46:BN:120:LEU:CD1  | 46:BN:122:VAL:HG23 | 2.38                     | 0.54              |
| 46:BN:55:VAL:HG22  | 46:BN:56:ASN:H     | 1.72                     | 0.54              |
| 48:BP:100:LEU:HA   | 48:BP:103:ALA:HB3  | 1.89                     | 0.54              |
| 51:BS:98:VAL:C     | 51:BS:100:ALA:N    | 2.60                     | 0.54              |
| 55:BW:9:TYR:H      | 55:BW:102:HIS:CD2  | 2.26                     | 0.54              |
| 58:BZ:145:GLU:O    | 58:BZ:147:GLY:N    | 2.40                     | 0.54              |
| 1:CA:10:A:H2'      | 1:CA:11:G:H8       | 1.72                     | 0.54              |
| 1:CA:675:A:O2'     | 1:CA:676:A:H5'     | 2.07                     | 0.54              |
| 1:CA:956:U:O2'     | 1:CA:957:U:H5'     | 2.08                     | 0.54              |
| 2:CB:187:LEU:HD23  | 2:CB:214:ILE:HG21  | 1.90                     | 0.54              |
| 3:CC:101:LEU:HD23  | 3:CC:101:LEU:C     | 2.28                     | 0.54              |
| 3:CC:59:ARG:CG     | 3:CC:64:VAL:HA     | 2.37                     | 0.54              |
| 5:CE:100:VAL:HG23  | 5:CE:100:VAL:O     | 2.07                     | 0.54              |
| 24:CY:92:ILE:HG13  | 24:CY:405:PRO:HG2  | 1.86                     | 0.54              |
| 35:DA:1344:G:H5'   | 35:DA:1384:A:C6    | 2.43                     | 0.54              |
| 35:DA:16:G:O2'     | 35:DA:17:G:H5'     | 2.07                     | 0.54              |
| 35:DA:1943:U:H4'   | 35:DA:1944:U:OP1   | 2.06                     | 0.54              |
| 35:DA:2142:C:O2'   | 35:DA:2143:C:H5'   | 2.08                     | 0.54              |
| 35:DA:737:C:C2'    | 35:DA:738:G:H5'    | 2.38                     | 0.54              |
| 35:DA:2202:C:H2'   | 38:DD:151:LYS:HZ1  | 1.71                     | 0.54              |
| 38:DD:155:LEU:N    | 38:DD:155:LEU:HD12 | 2.22                     | 0.54              |
| 40:DF:157:VAL:HG12 | 40:DF:176:LEU:HD23 | 1.89                     | 0.54              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 41:DG:46:ALA:HB2   | 41:DG:88:ILE:CG1  | 2.38                     | 0.54              |
| 47:DO:19:ILE:HD12  | 47:DO:41:ALA:HB3  | 1.90                     | 0.54              |
| 47:DO:47:ILE:O     | 47:DO:48:PRO:O    | 2.26                     | 0.54              |
| 1:AA:1030(C):G:H2' | 1:AA:1030(D):A:H8 | 1.71                     | 0.54              |
| 1:AA:1166:G:H5'    | 1:AA:1168:A:OP2   | 2.07                     | 0.54              |
| 1:AA:1226:C:H5''   | 13:AM:103:THR:CB  | 2.38                     | 0.54              |
| 3:AC:95:THR:O      | 3:AC:97:LYS:N     | 2.41                     | 0.54              |
| 4:AD:192:GLU:O     | 4:AD:193:ASP:C    | 2.45                     | 0.54              |
| 9:AI:4:TYR:CE2     | 9:AI:59:PHE:HE2   | 2.26                     | 0.54              |
| 24:AY:137:ASN:HD21 | 24:AY:263:ALA:H   | 1.55                     | 0.54              |
| 26:B1:29:GLY:C     | 26:B1:31:GLY:H    | 2.10                     | 0.54              |
| 26:B1:76:ARG:NH2   | 26:B1:95:LEU:HD13 | 2.23                     | 0.54              |
| 35:BA:2189:U:C3'   | 35:BA:2190:G:H5'' | 2.37                     | 0.54              |
| 35:BA:2577:A:C5'   | 35:BA:2578:G:H5'  | 2.37                     | 0.54              |
| 35:BA:2749:A:N1    | 35:BA:2750:A:N6   | 2.56                     | 0.54              |
| 35:BA:2870:C:H2'   | 35:BA:2871:C:O4'  | 2.07                     | 0.54              |
| 35:BA:64:A:H2'     | 35:BA:65:C:C6     | 2.43                     | 0.54              |
| 28:B3:45:GLY:HA3   | 35:BA:851:U:O2'   | 2.06                     | 0.54              |
| 35:BA:1824:G:OP1   | 38:BD:52:ARG:HD3  | 2.07                     | 0.54              |
| 38:BD:77:ALA:CB    | 38:BD:97:TYR:HA   | 2.37                     | 0.54              |
| 35:BA:322:A:H3'    | 40:BF:169:ASN:ND2 | 2.22                     | 0.54              |
| 41:BG:96:ARG:O     | 41:BG:97:ASP:HB2  | 2.08                     | 0.54              |
| 47:BO:108:GLU:OE2  | 47:BO:108:GLU:N   | 2.40                     | 0.54              |
| 52:BT:29:ARG:HG2   | 52:BT:85:LYS:CA   | 2.38                     | 0.54              |
| 53:BU:109:LEU:O    | 53:BU:112:ARG:HB2 | 2.07                     | 0.54              |
| 53:BU:83:LEU:HD12  | 53:BU:113:ALA:HB2 | 1.90                     | 0.54              |
| 57:BY:59:GLY:O     | 57:BY:60:PHE:HB2  | 2.07                     | 0.54              |
| 1:CA:1347:G:N2     | 1:CA:1373:G:H2'   | 2.22                     | 0.54              |
| 1:CA:393:A:O2'     | 1:CA:394:G:H5'    | 2.07                     | 0.54              |
| 1:CA:691:G:H2'     | 1:CA:692:U:C6     | 2.43                     | 0.54              |
| 2:CB:31:TYR:O      | 2:CB:42:ILE:HG13  | 2.08                     | 0.54              |
| 4:CD:61:LYS:CE     | 4:CD:62:GLN:HE21  | 2.21                     | 0.54              |
| 11:CK:122:LYS:O    | 11:CK:123:LYS:C   | 2.46                     | 0.54              |
| 13:CM:6:GLY:C      | 13:CM:8:GLU:N     | 2.59                     | 0.54              |
| 16:CP:4:ILE:HG13   | 16:CP:64:ALA:HB1  | 1.90                     | 0.54              |
| 20:CT:104:LEU:HD23 | 20:CT:104:LEU:C   | 2.28                     | 0.54              |
| 24:CY:112:GLN:HG3  | 24:CY:115:GLU:CB  | 2.37                     | 0.54              |
| 24:CY:689:LYS:HG3  | 24:CY:690:GLY:N   | 2.22                     | 0.54              |
| 26:D1:45:ASN:HB3   | 26:D1:64:ALA:HB2  | 1.89                     | 0.54              |
| 19:CS:42:PRO:HB3   | 29:D4:50:VAL:HG21 | 1.89                     | 0.54              |
| 33:D8:33:ASN:HA    | 33:D8:36:LYS:HG3  | 1.88                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:1493:C:O2    | 35:DA:1493:C:H2'   | 2.08                     | 0.54              |
| 35:DA:1972:A:H2'   | 35:DA:1973:G:H8    | 1.72                     | 0.54              |
| 35:DA:2336:A:N3    | 35:DA:2385:C:H1'   | 2.23                     | 0.54              |
| 35:DA:2617:C:O2'   | 35:DA:2618:G:H5'   | 2.07                     | 0.54              |
| 35:DA:2820:A:C8    | 39:DE:191:PRO:HB2  | 2.42                     | 0.54              |
| 35:DA:68:G:H2'     | 35:DA:69:C:C6      | 2.43                     | 0.54              |
| 36:DB:66:A:N6      | 36:DB:108:U:H2'    | 2.22                     | 0.54              |
| 38:DD:27:THR:HG23  | 38:DD:27:THR:O     | 2.07                     | 0.54              |
| 35:DA:1824:G:OP1   | 38:DD:52:ARG:HD3   | 2.08                     | 0.54              |
| 40:DF:9:ILE:HG12   | 40:DF:15:SER:N     | 2.22                     | 0.54              |
| 46:DN:66:LYS:O     | 46:DN:67:LEU:HD23  | 2.08                     | 0.54              |
| 48:DP:101:VAL:HA   | 48:DP:107:LYS:H    | 1.72                     | 0.54              |
| 48:DP:9:ASN:H      | 48:DP:10:PRO:CD    | 2.21                     | 0.54              |
| 49:DQ:27:VAL:HG12  | 49:DQ:28:ALA:N     | 2.21                     | 0.54              |
| 50:DR:85:PRO:C     | 50:DR:87:TYR:H     | 2.10                     | 0.54              |
| 52:DT:25:GLY:HA2   | 52:DT:92:GLY:HA2   | 1.90                     | 0.54              |
| 55:DW:25:ARG:NH2   | 55:DW:74:ALA:O     | 2.40                     | 0.54              |
| 4:AD:11:LEU:O      | 4:AD:12:CYS:C      | 2.45                     | 0.54              |
| 7:AG:81:GLY:O      | 7:AG:83:ALA:N      | 2.40                     | 0.54              |
| 7:AG:91:VAL:HG12   | 7:AG:92:SER:H      | 1.73                     | 0.54              |
| 9:AI:8:GLY:CA      | 9:AI:79:LEU:HD12   | 2.36                     | 0.54              |
| 9:AI:95:LYS:HD3    | 9:AI:95:LYS:C      | 2.28                     | 0.54              |
| 13:AM:11:ARG:HG2   | 13:AM:12:ASN:H     | 1.73                     | 0.54              |
| 13:AM:52:GLU:HA    | 13:AM:55:ARG:HD3   | 1.90                     | 0.54              |
| 13:AM:70:LEU:HD23  | 13:AM:70:LEU:C     | 2.27                     | 0.54              |
| 15:AO:9:GLN:HB3    | 15:AO:13:GLN:NE2   | 2.21                     | 0.54              |
| 17:AQ:45:HIS:CB    | 17:AQ:65:ILE:HD13  | 2.37                     | 0.54              |
| 19:AS:44:MET:HB3   | 19:AS:47:HIS:HD2   | 1.72                     | 0.54              |
| 20:AT:104:LEU:C    | 20:AT:104:LEU:HD23 | 2.27                     | 0.54              |
| 22:AW:52:C:H3'     | 22:AW:53:G:H5''    | 1.89                     | 0.54              |
| 22:AW:75:C:O2'     | 22:AW:76:C:H5'     | 2.07                     | 0.54              |
| 24:AY:227:ILE:HD11 | 24:AY:241:GLU:C    | 2.28                     | 0.54              |
| 34:B9:29:ASN:HD21  | 34:B9:32:HIS:CG    | 2.26                     | 0.54              |
| 35:BA:1197:G:H2'   | 35:BA:1198:U:H6    | 1.72                     | 0.54              |
| 35:BA:1943:U:O2'   | 35:BA:1944:U:H3'   | 2.08                     | 0.54              |
| 35:BA:1972:A:H2'   | 35:BA:1973:G:H8    | 1.73                     | 0.54              |
| 35:BA:2422:A:H4'   | 35:BA:2423:U:OP1   | 2.08                     | 0.54              |
| 35:BA:2465:C:O2'   | 35:BA:2466:C:H5'   | 2.08                     | 0.54              |
| 35:BA:653:A:H5'    | 35:BA:654:A:OP2    | 2.08                     | 0.54              |
| 35:BA:654(G):C:H2' | 35:BA:654(H):G:C8  | 2.38                     | 0.54              |
| 36:BB:35:U:O2      | 36:BB:35:U:H2'     | 2.07                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:BC:26:ALA:O     | 37:BC:30:VAL:HG23  | 2.07                     | 0.54              |
| 37:BC:73:VAL:CG1   | 37:BC:158:LYS:HA   | 2.38                     | 0.54              |
| 39:BE:70:ALA:O     | 39:BE:71:GLY:C     | 2.45                     | 0.54              |
| 39:BE:94:GLU:OE2   | 39:BE:177:PRO:HB3  | 2.07                     | 0.54              |
| 40:BF:10:PRO:HG2   | 40:BF:13:SER:OG    | 2.08                     | 0.54              |
| 40:BF:176:LEU:HG   | 40:BF:177:ALA:O    | 2.07                     | 0.54              |
| 48:BP:16:ARG:CD    | 48:BP:18:ARG:H     | 2.10                     | 0.54              |
| 48:BP:64:LYS:C     | 48:BP:66:GLY:H     | 2.10                     | 0.54              |
| 53:BU:99:ALA:HB2   | 53:BU:106:PHE:CE1  | 2.43                     | 0.54              |
| 56:BX:35:THR:HG22  | 56:BX:37:THR:N     | 2.14                     | 0.54              |
| 1:CA:1015:A:H2'    | 1:CA:1016:A:C8     | 2.43                     | 0.54              |
| 1:CA:1226:C:H4'    | 1:CA:1227:A:OP1    | 2.06                     | 0.54              |
| 1:CA:1258:G:O2'    | 1:CA:1259:C:H5'    | 2.07                     | 0.54              |
| 2:CB:137:ARG:HD3   | 2:CB:137:ARG:C     | 2.28                     | 0.54              |
| 4:CD:31:CYS:O      | 4:CD:32:ALA:HB3    | 2.08                     | 0.54              |
| 7:CG:69:VAL:HG21   | 7:CG:104:LEU:HD21  | 1.90                     | 0.54              |
| 10:CJ:33:GLN:N     | 10:CJ:75:ILE:HD11  | 2.22                     | 0.54              |
| 11:CK:20:TYR:HB2   | 11:CK:31:THR:HG22  | 1.90                     | 0.54              |
| 13:CM:56:LEU:C     | 13:CM:56:LEU:HD13  | 2.28                     | 0.54              |
| 17:CQ:45:HIS:CB    | 17:CQ:65:ILE:HD13  | 2.38                     | 0.54              |
| 19:CS:13:ASP:O     | 19:CS:15:LEU:N     | 2.40                     | 0.54              |
| 19:CS:53:ASN:O     | 19:CS:55:LYS:N     | 2.37                     | 0.54              |
| 24:CY:309:LEU:HD13 | 24:CY:334:THR:O    | 2.07                     | 0.54              |
| 25:D0:78:TYR:N     | 25:D0:78:TYR:CD1   | 2.75                     | 0.54              |
| 31:D6:27:LYS:CD    | 31:D6:27:LYS:O     | 2.54                     | 0.54              |
| 31:D6:13:CYS:HA    | 31:D6:50:ARG:O     | 2.08                     | 0.54              |
| 35:DA:2224:G:H4'   | 35:DA:2226:C:C2    | 2.43                     | 0.54              |
| 35:DA:2792:G:N3    | 35:DA:2792:G:H2'   | 2.23                     | 0.54              |
| 35:DA:2861:G:H2'   | 35:DA:2862:G:H8    | 1.72                     | 0.54              |
| 35:DA:648:G:H2'    | 35:DA:649:G:H8     | 1.71                     | 0.54              |
| 35:DA:709:U:H2'    | 35:DA:710:G:C8     | 2.42                     | 0.54              |
| 35:DA:83:G:O2'     | 35:DA:84:A:C8      | 2.56                     | 0.54              |
| 36:DB:49:C:H2'     | 36:DB:50:G:C8      | 2.43                     | 0.54              |
| 37:DC:76:LEU:HD21  | 37:DC:104:ILE:HD11 | 1.89                     | 0.54              |
| 38:DD:134:ARG:HG2  | 38:DD:187:GLY:O    | 2.07                     | 0.54              |
| 39:DE:4:ILE:HG13   | 39:DE:5:LEU:H      | 1.73                     | 0.54              |
| 41:DG:19:LEU:CD1   | 41:DG:172:LEU:HD12 | 2.38                     | 0.54              |
| 43:DJ:31:UNK:O     | 43:DJ:32:UNK:CB    | 2.56                     | 0.54              |
| 44:DK:109:LYS:HA   | 44:DK:112:MET:HE3  | 1.90                     | 0.54              |
| 35:DA:1059:G:H4'   | 44:DK:115:LEU:HD23 | 1.88                     | 0.54              |
| 48:DP:102:ARG:HG2  | 48:DP:102:ARG:O    | 2.07                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:DP:99:LEU:HA    | 48:DP:102:ARG:HH12 | 1.72                     | 0.54              |
| 48:DP:146:VAL:O    | 48:DP:148:LEU:HD12 | 2.08                     | 0.54              |
| 48:DP:9:ASN:N      | 48:DP:10:PRO:HD2   | 2.23                     | 0.54              |
| 30:D5:55:ARG:HH12  | 50:DR:33:ARG:CD    | 2.20                     | 0.54              |
| 35:DA:1654:A:P     | 50:DR:3:HIS:HB2    | 2.47                     | 0.54              |
| 52:DT:117:ASP:OD2  | 52:DT:120:ARG:HG3  | 2.08                     | 0.54              |
| 35:DA:483:A:H4'    | 57:DY:49:VAL:HA    | 1.90                     | 0.54              |
| 58:DZ:13:GLU:O     | 58:DZ:18:LEU:HD11  | 2.07                     | 0.54              |
| 1:AA:174:C:O2'     | 1:AA:175:C:H5'     | 2.08                     | 0.54              |
| 1:AA:179:A:H2'     | 1:AA:180:U:H6      | 1.70                     | 0.54              |
| 1:AA:261:U:O2      | 1:AA:263:A:C8      | 2.60                     | 0.54              |
| 1:AA:415:A:H2'     | 1:AA:416:G:C8      | 2.42                     | 0.54              |
| 1:AA:424:G:H2'     | 1:AA:425:G:H8      | 1.72                     | 0.54              |
| 2:AB:19:HIS:HD2    | 2:AB:189:ASP:OD2   | 1.90                     | 0.54              |
| 2:AB:207:ALA:O     | 2:AB:211:ILE:HG13  | 2.08                     | 0.54              |
| 3:AC:23:TYR:CG     | 3:AC:24:ALA:N      | 2.76                     | 0.54              |
| 4:AD:153:ARG:HG2   | 4:AD:153:ARG:HH11  | 1.71                     | 0.54              |
| 6:AF:8:ILE:HG23    | 6:AF:85:VAL:HG13   | 1.89                     | 0.54              |
| 10:AJ:58:ASP:O     | 10:AJ:59:SER:C     | 2.45                     | 0.54              |
| 13:AM:10:PRO:CG    | 13:AM:18:ALA:HB1   | 2.38                     | 0.54              |
| 16:AP:28:ARG:HG2   | 16:AP:28:ARG:HH11  | 1.72                     | 0.54              |
| 16:AP:43:LYS:HA    | 16:AP:48:TRP:CB    | 2.37                     | 0.54              |
| 24:AY:122:TRP:C    | 24:AY:124:GLN:N    | 2.61                     | 0.54              |
| 26:B1:86:SER:HA    | 26:B1:89:GLU:OE2   | 2.08                     | 0.54              |
| 31:B6:41:PRO:O     | 31:B6:42:TRP:C     | 2.47                     | 0.54              |
| 35:BA:1599:C:H2'   | 35:BA:1600:C:C6    | 2.41                     | 0.54              |
| 35:BA:41:C:H2'     | 35:BA:42:G:O4'     | 2.06                     | 0.54              |
| 35:BA:545:C:H2'    | 35:BA:547:A:C5'    | 2.32                     | 0.54              |
| 35:BA:615:G:OP2    | 40:BF:40:GLN:NE2   | 2.40                     | 0.54              |
| 40:BF:154:VAL:HG11 | 40:BF:193:VAL:CG2  | 2.38                     | 0.54              |
| 41:BG:16:ARG:O     | 41:BG:20:ILE:HG13  | 2.08                     | 0.54              |
| 47:BO:19:ILE:HD12  | 47:BO:41:ALA:HB3   | 1.90                     | 0.54              |
| 51:BS:20:ARG:HA    | 51:BS:20:ARG:NE    | 2.20                     | 0.54              |
| 1:CA:1130:A:C2     | 1:CA:1146:A:C4     | 2.96                     | 0.54              |
| 1:CA:1090:U:C4'    | 1:CA:1170:A:H2     | 2.21                     | 0.54              |
| 1:CA:1270:C:H2'    | 1:CA:1271:G:H8     | 1.71                     | 0.54              |
| 3:CC:94:LEU:HD12   | 3:CC:94:LEU:O      | 2.08                     | 0.54              |
| 1:CA:1368:G:OP2    | 9:CI:112:LYS:HD3   | 2.08                     | 0.54              |
| 9:CI:24:GLY:HA2    | 9:CI:59:PHE:O      | 2.07                     | 0.54              |
| 14:CN:47:LEU:O     | 14:CN:50:LYS:N     | 2.40                     | 0.54              |
| 19:CS:41:VAL:HG23  | 19:CS:41:VAL:O     | 2.08                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 19:CS:6:LYS:HE3     | 19:CS:6:LYS:H      | 1.72                     | 0.54              |
| 24:CY:272:LEU:HA    | 24:CY:275:ALA:HB3  | 1.90                     | 0.54              |
| 24:CY:505:GLY:HA3   | 24:CY:576:ASP:CB   | 2.38                     | 0.54              |
| 26:D1:82:LEU:O      | 26:D1:83:GLU:HG3   | 2.07                     | 0.54              |
| 29:D4:48:ARG:O      | 29:D4:49:PHE:CD1   | 2.61                     | 0.54              |
| 30:D5:35:GLU:O      | 30:D5:36:CYS:HB3   | 2.08                     | 0.54              |
| 31:D6:54:ILE:O      | 31:D6:54:ILE:CD1   | 2.53                     | 0.54              |
| 35:DA:1142(A):A:O2' | 35:DA:1143:A:H5''  | 2.06                     | 0.54              |
| 35:DA:1272:A:OP2    | 35:DA:1647:G:OP1   | 2.24                     | 0.54              |
| 35:DA:1902:C:H2'    | 35:DA:1903:G:O4'   | 2.07                     | 0.54              |
| 35:DA:2312:U:H2'    | 35:DA:2313:C:C5'   | 2.35                     | 0.54              |
| 35:DA:2469:A:H2     | 35:DA:2481:G:N2    | 2.06                     | 0.54              |
| 35:DA:2688:U:H1'    | 35:DA:2721:A:N6    | 2.23                     | 0.54              |
| 35:DA:2750:A:H2'    | 35:DA:2752:C:N4    | 2.22                     | 0.54              |
| 29:D4:2:LYS:CB      | 36:DB:40:U:O4      | 2.55                     | 0.54              |
| 37:DC:138:LEU:HD13  | 37:DC:139:PRO:O    | 2.08                     | 0.54              |
| 40:DF:25:PRO:CG     | 40:DF:119:ARG:HB2  | 2.37                     | 0.54              |
| 40:DF:181:LEU:HB3   | 40:DF:205:ARG:HH12 | 1.71                     | 0.54              |
| 40:DF:84:VAL:CG1    | 40:DF:85:GLY:N     | 2.55                     | 0.54              |
| 41:DG:120:LEU:HD12  | 41:DG:180:PHE:CE2  | 2.43                     | 0.54              |
| 46:DN:94:HIS:N      | 46:DN:95:PRO:CD    | 2.71                     | 0.54              |
| 49:DQ:45:GLN:H      | 49:DQ:45:GLN:HE21  | 1.52                     | 0.54              |
| 53:DU:109:LEU:O     | 53:DU:112:ARG:HB2  | 2.07                     | 0.54              |
| 53:DU:12:ARG:HB3    | 53:DU:16:LYS:HE3   | 1.90                     | 0.54              |
| 55:DW:20:VAL:HG23   | 55:DW:21:VAL:N     | 2.23                     | 0.54              |
| 56:DX:12:VAL:CG1    | 56:DX:27:THR:HG23  | 2.35                     | 0.54              |
| 56:DX:18:TYR:O      | 56:DX:20:GLY:N     | 2.41                     | 0.54              |
| 57:DY:67:LEU:HD11   | 57:DY:71:LYS:HE2   | 1.89                     | 0.54              |
| 58:DZ:80:ARG:O      | 58:DZ:81:ARG:C     | 2.46                     | 0.54              |
| 1:AA:1060:C:H5'     | 14:AN:45:ARG:NH2   | 2.23                     | 0.54              |
| 1:AA:1459:C:H2'     | 1:AA:1460:A:H8     | 1.73                     | 0.54              |
| 1:AA:781:A:H2'      | 1:AA:782:A:H5'     | 1.89                     | 0.54              |
| 2:AB:17:PHE:O       | 2:AB:204:ASN:HB2   | 2.08                     | 0.54              |
| 2:AB:209:ARG:NH1    | 2:AB:239:VAL:HG11  | 2.23                     | 0.54              |
| 19:AS:43:GLU:O      | 19:AS:45:VAL:HG13  | 2.08                     | 0.54              |
| 24:AY:546:ILE:CG2   | 24:AY:590:ILE:HG13 | 2.27                     | 0.54              |
| 29:B4:10:VAL:N      | 29:B4:26:SER:O     | 2.41                     | 0.54              |
| 35:BA:2818:G:O2'    | 35:BA:2837:G:H5'   | 2.08                     | 0.54              |
| 35:BA:67:U:H2'      | 35:BA:68:G:C8      | 2.43                     | 0.54              |
| 35:BA:883:G:O2'     | 35:BA:884:C:H5'    | 2.07                     | 0.54              |
| 35:BA:892:G:H2'     | 35:BA:893:C:H6     | 1.73                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BB:94:C:H2'     | 36:BB:95:C:H6      | 1.73                     | 0.54              |
| 37:BC:127:LYS:O    | 37:BC:128:LEU:HG   | 2.08                     | 0.54              |
| 38:BD:71:ASP:CB    | 38:BD:103:ARG:HH22 | 2.07                     | 0.54              |
| 35:BA:1568:G:OP2   | 38:BD:63:ARG:NH2   | 2.37                     | 0.54              |
| 38:BD:79:VAL:O     | 38:BD:113:VAL:HG13 | 2.08                     | 0.54              |
| 39:BE:95:ILE:HD13  | 39:BE:95:ILE:N     | 2.23                     | 0.54              |
| 40:BF:18:ARG:C     | 40:BF:19:GLU:HG2   | 2.28                     | 0.54              |
| 46:BN:14:VAL:HG13  | 46:BN:137:LYS:HG3  | 1.90                     | 0.54              |
| 47:BO:26:LYS:HB3   | 47:BO:30:ALA:CB    | 2.37                     | 0.54              |
| 30:B5:55:ARG:NH2   | 50:BR:113:LEU:HD21 | 2.23                     | 0.54              |
| 52:BT:98:LYS:HB3   | 52:BT:100:TYR:CE1  | 2.43                     | 0.54              |
| 55:BW:80:PRO:O     | 55:BW:100:THR:HG21 | 2.08                     | 0.54              |
| 58:BZ:29:TYR:O     | 58:BZ:30:ASN:HB3   | 2.07                     | 0.54              |
| 1:CA:25:C:H2'      | 1:CA:26:A:C8       | 2.43                     | 0.54              |
| 1:CA:603:U:H2'     | 1:CA:604:G:C8      | 2.43                     | 0.54              |
| 1:CA:896:C:O2'     | 1:CA:897:C:H5'     | 2.07                     | 0.54              |
| 1:CA:945:G:C2      | 1:CA:946:A:C8      | 2.96                     | 0.54              |
| 1:CA:977:A:C2'     | 1:CA:978:A:H5'     | 2.37                     | 0.54              |
| 2:CB:9:GLU:OE2     | 2:CB:9:GLU:N       | 2.40                     | 0.54              |
| 4:CD:129:ASN:N     | 4:CD:129:ASN:HD22  | 2.06                     | 0.54              |
| 6:CF:42:GLU:C      | 6:CF:44:GLY:H      | 2.11                     | 0.54              |
| 9:CI:128:ARG:O     | 13:CM:125:ARG:HD2  | 2.08                     | 0.54              |
| 9:CI:18:PHE:O      | 9:CI:61:ALA:HA     | 2.08                     | 0.54              |
| 11:CK:111:ASP:HA   | 18:CR:84:LYS:CD    | 2.31                     | 0.54              |
| 13:CM:124:PRO:HG2  | 24:CY:574:GLU:N    | 2.08                     | 0.54              |
| 1:CA:264:U:H4'     | 17:CQ:63:ARG:HD3   | 1.89                     | 0.54              |
| 24:CY:211:GLU:HB2  | 24:CY:215:LYS:NZ   | 2.23                     | 0.54              |
| 24:CY:322:VAL:HG23 | 24:CY:323:GLY:N    | 2.23                     | 0.54              |
| 25:D0:40:GLN:NE2   | 25:D0:43:THR:CA    | 2.67                     | 0.54              |
| 26:D1:20:ARG:HH11  | 26:D1:20:ARG:HG2   | 1.73                     | 0.54              |
| 35:DA:1441:G:H2'   | 35:DA:1442:G:C8    | 2.42                     | 0.54              |
| 35:DA:1754:C:OP1   | 52:DT:96:ARG:NH1   | 2.40                     | 0.54              |
| 35:DA:1840:G:H1    | 35:DA:1902:C:H42   | 1.56                     | 0.54              |
| 35:DA:2713:A:C3'   | 35:DA:2714:G:H5'   | 2.38                     | 0.54              |
| 35:DA:810:U:OP1    | 35:DA:1253:A:N7    | 2.40                     | 0.54              |
| 37:DC:225:ILE:O    | 37:DC:225:ILE:HD12 | 2.08                     | 0.54              |
| 39:DE:4:ILE:CG1    | 39:DE:5:LEU:N      | 2.71                     | 0.54              |
| 40:DF:25:PRO:HB2   | 40:DF:119:ARG:HD3  | 1.89                     | 0.54              |
| 40:DF:84:VAL:CG1   | 40:DF:85:GLY:H     | 2.12                     | 0.54              |
| 41:DG:98:ARG:HH11  | 41:DG:98:ARG:CG    | 2.20                     | 0.54              |
| 48:DP:47:ASP:HB3   | 48:DP:48:PRO:O     | 2.08                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:D5:55:ARG:NH2   | 50:DR:113:LEU:HD21 | 2.23                     | 0.54              |
| 57:DY:74:PRO:O     | 57:DY:75:ILE:HB    | 2.07                     | 0.54              |
| 58:DZ:95:PRO:HA    | 58:DZ:128:VAL:O    | 2.08                     | 0.54              |
| 1:AA:1316:G:N2     | 1:AA:1318:A:H3'    | 2.23                     | 0.54              |
| 1:AA:624:C:O2'     | 1:AA:625:G:H5'     | 2.07                     | 0.54              |
| 1:AA:1080:A:H5''   | 5:AE:16:THR:HG21   | 1.89                     | 0.54              |
| 6:AF:7:ASN:OD1     | 6:AF:62:TRP:HD1    | 1.91                     | 0.54              |
| 8:AH:103:VAL:HG23  | 8:AH:110:ALA:HB2   | 1.88                     | 0.54              |
| 8:AH:31:PHE:O      | 8:AH:34:GLU:HB2    | 2.08                     | 0.54              |
| 10:AJ:75:ILE:CG1   | 10:AJ:76:ASN:H     | 2.06                     | 0.54              |
| 13:AM:116:THR:HG22 | 13:AM:117:VAL:N    | 2.23                     | 0.54              |
| 18:AR:56:THR:O     | 18:AR:58:LEU:HD12  | 2.07                     | 0.54              |
| 24:AY:238:THR:HG23 | 24:AY:241:GLU:H    | 1.72                     | 0.54              |
| 27:B2:15:LYS:O     | 27:B2:16:LEU:HD23  | 2.08                     | 0.54              |
| 28:B3:4:LEU:O      | 28:B3:36:VAL:HA    | 2.08                     | 0.54              |
| 31:B6:11:LEU:CG    | 31:B6:26:ASN:HD21  | 2.21                     | 0.54              |
| 32:B7:24:THR:HG23  | 32:B7:27:GLY:CA    | 2.38                     | 0.54              |
| 35:BA:1036:G:C6    | 35:BA:1120:G:C6    | 2.96                     | 0.54              |
| 35:BA:1173:G:H5'   | 35:BA:1174:A:O5'   | 2.07                     | 0.54              |
| 35:BA:1287:A:H2'   | 35:BA:1287:A:N3    | 2.21                     | 0.54              |
| 35:BA:2183:C:O2'   | 35:BA:2184:G:H5'   | 2.08                     | 0.54              |
| 35:BA:2469:A:H2    | 35:BA:2481:G:N2    | 2.05                     | 0.54              |
| 35:BA:2521:C:N4    | 35:BA:2544:G:H1    | 2.06                     | 0.54              |
| 35:BA:491:G:H2'    | 35:BA:492:A:C8     | 2.42                     | 0.54              |
| 37:BC:138:LEU:HD13 | 37:BC:139:PRO:O    | 2.07                     | 0.54              |
| 37:BC:57:GLN:NE2   | 37:BC:205:ALA:HA   | 2.22                     | 0.54              |
| 38:BD:5:LYS:HD2    | 38:BD:17:THR:HG22  | 1.89                     | 0.54              |
| 40:BF:124:LEU:HD22 | 40:BF:191:ARG:HH21 | 1.73                     | 0.54              |
| 46:BN:15:LEU:HD12  | 46:BN:136:GLU:HG3  | 1.90                     | 0.54              |
| 46:BN:96:GLU:N     | 46:BN:96:GLU:CD    | 2.57                     | 0.54              |
| 48:BP:47:ASP:HB2   | 48:BP:51:PHE:HB2   | 1.90                     | 0.54              |
| 49:BQ:108:GLY:O    | 49:BQ:109:VAL:CG2  | 2.56                     | 0.54              |
| 51:BS:56:LEU:O     | 51:BS:56:LEU:HD23  | 2.08                     | 0.54              |
| 30:B5:27:PRO:HG3   | 55:BW:23:LEU:CD1   | 2.35                     | 0.54              |
| 56:BX:65:ARG:HH11  | 56:BX:65:ARG:HG2   | 1.72                     | 0.54              |
| 35:BA:302:C:P      | 57:BY:73:ARG:HH12  | 2.31                     | 0.54              |
| 57:BY:95:LYS:CD    | 57:BY:101:LYS:H    | 2.21                     | 0.54              |
| 58:BZ:126:VAL:HG23 | 58:BZ:127:LYS:N    | 2.23                     | 0.54              |
| 1:CA:1221:G:H4'    | 19:CS:77:THR:CG2   | 2.35                     | 0.54              |
| 1:CA:383:A:C2'     | 1:CA:384:G:H5'     | 2.38                     | 0.54              |
| 1:CA:542:G:H5'     | 4:CD:41:GLY:CA     | 2.37                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:CB:204:ASN:HD21  | 2:CB:206:ASP:H     | 1.54                     | 0.54              |
| 5:CE:43:LEU:HD21   | 5:CE:132:ALA:HB1   | 1.89                     | 0.54              |
| 7:CG:64:GLN:HG3    | 7:CG:128:ALA:HB1   | 1.91                     | 0.54              |
| 19:CS:72:GLY:O     | 19:CS:74:PHE:N     | 2.41                     | 0.54              |
| 13:CM:94:ARG:NE    | 19:CS:82:GLY:N     | 2.56                     | 0.54              |
| 24:CY:124:GLN:HA   | 24:CY:127:LYS:HD2  | 1.89                     | 0.54              |
| 24:CY:152:THR:HG23 | 24:CY:153:MET:N    | 2.23                     | 0.54              |
| 24:CY:232:LEU:HD22 | 24:CY:232:LEU:H    | 1.73                     | 0.54              |
| 24:CY:331:TYR:O    | 24:CY:371:ALA:CB   | 2.56                     | 0.54              |
| 35:DA:1044:G:O2'   | 35:DA:1045:A:H5''  | 2.07                     | 0.54              |
| 35:DA:1358:G:O2'   | 35:DA:1359:A:H5''  | 2.08                     | 0.54              |
| 35:DA:648:G:H2'    | 35:DA:649:G:C8     | 2.43                     | 0.54              |
| 35:DA:654(P):C:H2' | 35:DA:654(Q):C:H5' | 1.90                     | 0.54              |
| 35:DA:863:A:O2'    | 36:DB:101:G:H1'    | 2.08                     | 0.54              |
| 38:DD:30:GLU:HG3   | 38:DD:63:ARG:CZ    | 2.38                     | 0.54              |
| 40:DF:7:TYR:OH     | 40:DF:10:PRO:HG3   | 2.06                     | 0.54              |
| 46:DN:24:GLY:HA2   | 46:DN:27:ALA:HB3   | 1.90                     | 0.54              |
| 48:DP:115:LEU:HD23 | 48:DP:115:LEU:H    | 1.72                     | 0.54              |
| 50:DR:7:GLY:HA3    | 50:DR:8:ARG:NH2    | 2.23                     | 0.54              |
| 50:DR:7:GLY:O      | 50:DR:8:ARG:CB     | 2.56                     | 0.54              |
| 52:DT:55:ASN:H     | 52:DT:59:THR:HG21  | 1.72                     | 0.54              |
| 56:DX:55:ASN:HB2   | 56:DX:80:ILE:HG12  | 1.90                     | 0.54              |
| 1:AA:1312:G:O2'    | 1:AA:1313:U:H5'    | 2.08                     | 0.53              |
| 1:AA:1516:G:H2'    | 1:AA:1518:A:OP2    | 2.08                     | 0.53              |
| 1:AA:255:G:O6      | 1:AA:266:G:O6      | 2.25                     | 0.53              |
| 1:AA:363:A:OP1     | 12:AL:33:ARG:HD3   | 2.08                     | 0.53              |
| 1:AA:781:A:H4'     | 1:AA:1522:U:O2'    | 2.09                     | 0.53              |
| 2:AB:86:GLU:C      | 2:AB:88:ALA:H      | 2.10                     | 0.53              |
| 3:AC:5:ILE:HD13    | 3:AC:5:ILE:O       | 2.08                     | 0.53              |
| 4:AD:31:CYS:O      | 4:AD:32:ALA:HB3    | 2.08                     | 0.53              |
| 10:AJ:78:ASN:C     | 10:AJ:79:ARG:HH11  | 2.11                     | 0.53              |
| 11:AK:108:ILE:CD1  | 11:AK:108:ILE:N    | 2.68                     | 0.53              |
| 13:AM:80:ARG:O     | 13:AM:83:ASP:HB3   | 2.08                     | 0.53              |
| 19:AS:53:ASN:C     | 19:AS:55:LYS:H     | 2.11                     | 0.53              |
| 19:AS:62:ILE:HG13  | 19:AS:62:ILE:O     | 2.08                     | 0.53              |
| 24:AY:498:ILE:HG22 | 24:AY:507:TYR:CD2  | 2.43                     | 0.53              |
| 24:AY:662:LYS:HZ2  | 42:BH:175:LYS:CG   | 2.21                     | 0.53              |
| 25:B0:40:GLN:NE2   | 25:B0:43:THR:CA    | 2.70                     | 0.53              |
| 26:B1:56:GLN:NE2   | 26:B1:56:GLN:HA    | 2.18                     | 0.53              |
| 27:B2:48:HIS:ND1   | 35:BA:95:G:O2'     | 2.40                     | 0.53              |
| 27:B2:32:LEU:HG    | 27:B2:53:LEU:HD13  | 1.90                     | 0.53              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 30:B5:7:PRO:HA    | 35:BA:2615:U:C2    | 2.43                     | 0.53              |
| 31:B6:9:LEU:O     | 31:B6:9:LEU:HD22   | 2.08                     | 0.53              |
| 34:B9:22:ARG:NH2  | 35:BA:2741:A:OP1   | 2.42                     | 0.53              |
| 35:BA:1050:A:C5   | 35:BA:1051:G:H1'   | 2.44                     | 0.53              |
| 35:BA:610:G:H22   | 35:BA:619:G:H1'    | 1.73                     | 0.53              |
| 35:BA:710:G:H2'   | 35:BA:711:G:C8     | 2.43                     | 0.53              |
| 36:BB:61:G:O2'    | 36:BB:62:C:H5'     | 2.08                     | 0.53              |
| 38:BD:209:ALA:C   | 38:BD:210:GLY:O    | 2.44                     | 0.53              |
| 38:BD:210:GLY:O   | 38:BD:212:SER:N    | 2.39                     | 0.53              |
| 38:BD:218:ARG:HG3 | 38:BD:218:ARG:HH11 | 1.73                     | 0.53              |
| 40:BF:113:ALA:HB1 | 40:BF:186:ILE:CG2  | 2.37                     | 0.53              |
| 41:BG:119:GLY:HA3 | 41:BG:181:ARG:N    | 2.23                     | 0.53              |
| 42:BH:46:GLU:HG3  | 42:BH:51:ARG:HB2   | 1.89                     | 0.53              |
| 35:BA:1107:G:OP1  | 43:BJ:59:UNK:N     | 2.41                     | 0.53              |
| 48:BP:101:VAL:HA  | 48:BP:107:LYS:H    | 1.73                     | 0.53              |
| 48:BP:16:ARG:O    | 48:BP:18:ARG:N     | 2.41                     | 0.53              |
| 49:BQ:116:GLU:O   | 49:BQ:120:ILE:HG12 | 2.08                     | 0.53              |
| 50:BR:55:ALA:HB2  | 50:BR:79:LEU:HD11  | 1.90                     | 0.53              |
| 52:BT:11:GLU:O    | 52:BT:13:ARG:N     | 2.36                     | 0.53              |
| 53:BU:113:ALA:C   | 53:BU:115:ALA:N    | 2.61                     | 0.53              |
| 53:BU:61:TRP:HB3  | 53:BU:93:LYS:HB3   | 1.89                     | 0.53              |
| 54:BV:66:ARG:CZ   | 54:BV:88:ARG:HH21  | 2.21                     | 0.53              |
| 56:BX:18:TYR:O    | 56:BX:20:GLY:N     | 2.41                     | 0.53              |
| 1:CA:1307:U:H2'   | 1:CA:1308:U:C6     | 2.43                     | 0.53              |
| 1:CA:737:A:H2'    | 1:CA:738:C:H6      | 1.73                     | 0.53              |
| 3:CC:59:ARG:HD3   | 3:CC:64:VAL:HG22   | 1.90                     | 0.53              |
| 8:CH:103:VAL:HG21 | 8:CH:110:ALA:HB2   | 1.90                     | 0.53              |
| 9:CI:84:ALA:C     | 9:CI:86:VAL:H      | 2.11                     | 0.53              |
| 13:CM:66:LEU:O    | 13:CM:70:LEU:HB3   | 2.08                     | 0.53              |
| 15:CO:64:ARG:HH11 | 15:CO:64:ARG:HG3   | 1.73                     | 0.53              |
| 16:CP:43:LYS:HA   | 16:CP:48:TRP:CB    | 2.37                     | 0.53              |
| 24:CY:600:VAL:O   | 24:CY:600:VAL:HG13 | 2.08                     | 0.53              |
| 24:CY:679:VAL:O   | 24:CY:681:LYS:N    | 2.41                     | 0.53              |
| 27:D2:35:LEU:HD12 | 27:D2:53:LEU:HD12  | 1.89                     | 0.53              |
| 31:D6:15:GLU:CD   | 31:D6:44:ARG:NH2   | 2.62                     | 0.53              |
| 35:DA:1092:C:H2'  | 35:DA:1093:G:H8    | 1.72                     | 0.53              |
| 35:DA:1252:G:N3   | 53:DU:33:ARG:HD2   | 2.22                     | 0.53              |
| 35:DA:1291:C:H2'  | 35:DA:1292:U:C6    | 2.43                     | 0.53              |
| 35:DA:1305:C:O2'  | 35:DA:1306:C:H5'   | 2.08                     | 0.53              |
| 35:DA:2076:U:H5'  | 35:DA:2238:G:N2    | 2.21                     | 0.53              |
| 35:DA:284:U:H2'   | 35:DA:285:C:C6     | 2.41                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:650:C:C3'    | 35:DA:651:G:H5''   | 2.37                     | 0.53              |
| 35:DA:816:C:O2'    | 35:DA:817:C:H5'    | 2.08                     | 0.53              |
| 40:DF:81:PRO:O     | 40:DF:83:PHE:N     | 2.41                     | 0.53              |
| 41:DG:34:LEU:HD11  | 41:DG:100:TRP:CH2  | 2.43                     | 0.53              |
| 43:DJ:20:UNK:CB    | 43:DJ:88:UNK:O     | 2.56                     | 0.53              |
| 35:DA:1063:G:O2'   | 44:DK:87:GLY:HA3   | 2.07                     | 0.53              |
| 48:DP:122:PRO:O    | 48:DP:123:LEU:HB3  | 2.08                     | 0.53              |
| 1:AA:1030:C:H2'    | 1:AA:1030(A):G:H5' | 1.91                     | 0.53              |
| 1:AA:346:G:OP1     | 52:BT:41:ARG:CZ    | 2.56                     | 0.53              |
| 1:AA:893:C:H2'     | 1:AA:894:G:H8      | 1.74                     | 0.53              |
| 1:AA:956:U:O2'     | 1:AA:957:U:H5'     | 2.08                     | 0.53              |
| 6:AF:33:TYR:HA     | 6:AF:71:ARG:HH21   | 1.73                     | 0.53              |
| 10:AJ:4:ILE:HB     | 10:AJ:74:ILE:HD11  | 1.89                     | 0.53              |
| 15:AO:17:ARG:HH11  | 15:AO:17:ARG:HG3   | 1.73                     | 0.53              |
| 15:AO:76:GLU:C     | 15:AO:78:TYR:N     | 2.61                     | 0.53              |
| 22:AW:8:U:H1'      | 22:AW:49:C:H1'     | 1.90                     | 0.53              |
| 24:AY:213:HIS:O    | 24:AY:217:VAL:HG23 | 2.08                     | 0.53              |
| 24:AY:227:ILE:HG12 | 24:AY:237:PRO:HB3  | 1.90                     | 0.53              |
| 24:AY:637:ARG:HG3  | 24:AY:637:ARG:NH1  | 2.23                     | 0.53              |
| 31:B6:7:ILE:O      | 31:B6:27:LYS:HD3   | 2.08                     | 0.53              |
| 32:B7:24:THR:C     | 32:B7:26:GLY:H     | 2.11                     | 0.53              |
| 30:B5:19:ARG:HD2   | 35:BA:1266:G:OP1   | 2.08                     | 0.53              |
| 35:BA:2713:A:C3'   | 35:BA:2714:G:H5'   | 2.38                     | 0.53              |
| 35:BA:528:A:C2     | 35:BA:2043:C:H5'   | 2.44                     | 0.53              |
| 41:BG:46:ALA:HB2   | 41:BG:88:ILE:HG12  | 1.90                     | 0.53              |
| 43:BJ:48:UNK:O     | 43:BJ:49:UNK:O     | 2.27                     | 0.53              |
| 47:BO:34:THR:O     | 47:BO:35:VAL:C     | 2.45                     | 0.53              |
| 48:BP:85:LEU:CD2   | 48:BP:85:LEU:H     | 2.14                     | 0.53              |
| 50:BR:11:ASN:O     | 50:BR:12:ARG:HB2   | 2.07                     | 0.53              |
| 51:BS:14:VAL:O     | 51:BS:15:ARG:C     | 2.46                     | 0.53              |
| 53:BU:104:GLN:HB3  | 54:BV:44:LYS:NZ    | 2.23                     | 0.53              |
| 57:BY:86:ARG:HB3   | 57:BY:88:LYS:HZ1   | 1.72                     | 0.53              |
| 1:CA:1015:A:H2'    | 1:CA:1016:A:O4'    | 2.07                     | 0.53              |
| 1:CA:1208:C:H2'    | 1:CA:1209:C:H6     | 1.72                     | 0.53              |
| 1:CA:1258:G:H2'    | 1:CA:1259:C:C6     | 2.43                     | 0.53              |
| 1:CA:1521:G:H2'    | 1:CA:1522:U:C6     | 2.43                     | 0.53              |
| 1:CA:628:G:O2'     | 1:CA:629:G:H5'     | 2.07                     | 0.53              |
| 1:CA:950:U:H2'     | 1:CA:951:G:C8      | 2.43                     | 0.53              |
| 2:CB:17:PHE:O      | 2:CB:204:ASN:HB2   | 2.08                     | 0.53              |
| 2:CB:163:PHE:CD2   | 2:CB:185:ILE:HG13  | 2.42                     | 0.53              |
| 6:CF:80:ARG:NH1    | 6:CF:88:VAL:HB     | 2.23                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:CG:64:GLN:CG     | 7:CG:128:ALA:HB1   | 2.38                     | 0.53              |
| 7:CG:84:ASN:HD22   | 7:CG:84:ASN:N      | 2.06                     | 0.53              |
| 9:CI:81:ILE:O      | 9:CI:85:LEU:HG     | 2.07                     | 0.53              |
| 9:CI:4:TYR:CE2     | 9:CI:88:TYR:CB     | 2.91                     | 0.53              |
| 13:CM:78:ILE:CA    | 13:CM:81:LEU:HD23  | 2.38                     | 0.53              |
| 21:CU:3:LYS:HB3    | 21:CU:14:TRP:CD1   | 2.44                     | 0.53              |
| 24:CY:142:THR:O    | 24:CY:144:ALA:N    | 2.40                     | 0.53              |
| 24:CY:14:ASN:HD22  | 24:CY:14:ASN:N     | 2.04                     | 0.53              |
| 24:CY:131:PRO:CG   | 24:CY:281:PRO:HG3  | 2.34                     | 0.53              |
| 24:CY:343:ASN:HD22 | 24:CY:344:THR:N    | 2.07                     | 0.53              |
| 24:CY:416:LYS:CG   | 24:CY:417:THR:H    | 2.19                     | 0.53              |
| 24:CY:524:GLU:HG2  | 24:CY:524:GLU:O    | 2.08                     | 0.53              |
| 24:CY:601:ILE:HD12 | 24:CY:684:GLN:HG3  | 1.90                     | 0.53              |
| 26:D1:86:SER:HB3   | 26:D1:89:GLU:HB2   | 1.90                     | 0.53              |
| 35:DA:2688:U:H2'   | 35:DA:2719:G:N2    | 2.23                     | 0.53              |
| 35:DA:55:G:H2'     | 35:DA:56:A:C8      | 2.43                     | 0.53              |
| 35:DA:588:U:H2'    | 35:DA:589:C:H6     | 1.72                     | 0.53              |
| 35:DA:588:U:H2'    | 35:DA:589:C:C6     | 2.42                     | 0.53              |
| 35:DA:653:A:H5'    | 35:DA:654:A:OP2    | 2.08                     | 0.53              |
| 35:DA:710:G:H2'    | 35:DA:711:G:C8     | 2.43                     | 0.53              |
| 35:DA:881:G:C2'    | 35:DA:882:G:H5'    | 2.39                     | 0.53              |
| 40:DF:176:LEU:HG   | 40:DF:177:ALA:O    | 2.08                     | 0.53              |
| 44:DK:29:GLN:O     | 44:DK:59:ILE:HD12  | 2.08                     | 0.53              |
| 44:DK:5:VAL:HA     | 44:DK:59:ILE:CG2   | 2.37                     | 0.53              |
| 47:DO:105:GLU:O    | 47:DO:109:LYS:CG   | 2.56                     | 0.53              |
| 48:DP:64:LYS:C     | 48:DP:66:GLY:H     | 2.10                     | 0.53              |
| 48:DP:98:GLU:O     | 48:DP:101:VAL:HG22 | 2.09                     | 0.53              |
| 52:DT:98:LYS:HB3   | 52:DT:100:TYR:CE1  | 2.43                     | 0.53              |
| 52:DT:10:VAL:O     | 52:DT:13:ARG:HG2   | 2.08                     | 0.53              |
| 52:DT:35:LYS:HZ3   | 52:DT:41:ARG:NH1   | 2.05                     | 0.53              |
| 52:DT:3:ARG:O      | 52:DT:4:GLY:C      | 2.44                     | 0.53              |
| 54:DV:19:LYS:NZ    | 54:DV:20:LEU:H     | 2.05                     | 0.53              |
| 56:DX:27:THR:CB    | 56:DX:80:ILE:HG22  | 2.36                     | 0.53              |
| 57:DY:73:ARG:O     | 57:DY:74:PRO:O     | 2.26                     | 0.53              |
| 58:DZ:145:GLU:C    | 58:DZ:147:GLY:N    | 2.53                     | 0.53              |
| 1:AA:603:U:H2'     | 1:AA:604:G:C8      | 2.42                     | 0.53              |
| 2:AB:126:GLU:HA    | 2:AB:129:GLU:CD    | 2.27                     | 0.53              |
| 2:AB:151:GLY:O     | 2:AB:152:PHE:C     | 2.47                     | 0.53              |
| 2:AB:204:ASN:HD22  | 2:AB:206:ASP:H     | 1.51                     | 0.53              |
| 2:AB:221:LEU:O     | 2:AB:221:LEU:HD13  | 2.09                     | 0.53              |
| 6:AF:19:LEU:HD23   | 6:AF:19:LEU:C      | 2.28                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1152:A:H5''   | 10:AJ:13:HIS:HD2   | 1.73                     | 0.53              |
| 11:AK:105:VAL:HG23 | 11:AK:105:VAL:O    | 2.09                     | 0.53              |
| 12:AL:36:VAL:HG11  | 24:AY:425:SER:HB3  | 1.90                     | 0.53              |
| 29:B4:10:VAL:CG2   | 29:B4:11:PRO:HD2   | 2.34                     | 0.53              |
| 30:B5:50:GLY:HA2   | 30:B5:56:LYS:HB3   | 1.89                     | 0.53              |
| 35:BA:1151:G:H5''  | 53:BU:81:HIS:CE1   | 2.43                     | 0.53              |
| 35:BA:1505:C:C5    | 35:BA:1506:C:H1'   | 2.42                     | 0.53              |
| 35:BA:1803:A:O3'   | 38:BD:259:THR:CG2  | 2.51                     | 0.53              |
| 35:BA:1826:G:H4'   | 38:BD:242:ARG:NH2  | 2.19                     | 0.53              |
| 35:BA:1839:G:H2'   | 35:BA:1839:G:N3    | 2.24                     | 0.53              |
| 35:BA:528:A:H2     | 35:BA:2043:C:H5'   | 1.72                     | 0.53              |
| 35:BA:2118:U:OP1   | 35:BA:2148:G:H4'   | 2.08                     | 0.53              |
| 35:BA:2873:A:H4'   | 50:BR:8:ARG:NH2    | 2.23                     | 0.53              |
| 37:BC:139:PRO:HA   | 37:BC:145:THR:HB   | 1.90                     | 0.53              |
| 37:BC:213:VAL:CG1  | 37:BC:225:ILE:HD11 | 2.39                     | 0.53              |
| 39:BE:119:ARG:HG2  | 39:BE:160:TYR:HB2  | 1.90                     | 0.53              |
| 40:BF:62:ARG:NH2   | 40:BF:64:ILE:HA    | 2.24                     | 0.53              |
| 41:BG:133:LEU:HD12 | 41:BG:133:LEU:C    | 2.28                     | 0.53              |
| 42:BH:144:VAL:O    | 42:BH:148:ILE:HG12 | 2.08                     | 0.53              |
| 46:BN:87:LEU:O     | 46:BN:90:MET:N     | 2.41                     | 0.53              |
| 48:BP:75:ILE:N     | 48:BP:75:ILE:HD12  | 2.23                     | 0.53              |
| 48:BP:9:ASN:H      | 48:BP:10:PRO:CD    | 2.21                     | 0.53              |
| 36:BB:49:C:OP1     | 51:BS:96:GLY:HA3   | 2.07                     | 0.53              |
| 54:BV:49:THR:O     | 54:BV:50:PRO:C     | 2.46                     | 0.53              |
| 57:BY:95:LYS:HE2   | 57:BY:101:LYS:H    | 1.74                     | 0.53              |
| 1:CA:1008:C:H2'    | 1:CA:1009:G:H8     | 1.72                     | 0.53              |
| 1:CA:1458:G:OP1    | 20:CT:35:THR:HG21  | 2.08                     | 0.53              |
| 1:CA:189(K):U:H2'  | 1:CA:189(L):G:C8   | 2.43                     | 0.53              |
| 1:CA:268:C:O2      | 1:CA:268:C:H2'     | 2.08                     | 0.53              |
| 1:CA:423:G:H2'     | 1:CA:424:G:H5'     | 1.89                     | 0.53              |
| 1:CA:973:G:H1'     | 10:CJ:55:LYS:HZ3   | 1.73                     | 0.53              |
| 2:CB:97:TRP:HH2    | 2:CB:176:GLU:CD    | 2.12                     | 0.53              |
| 3:CC:5:ILE:HD13    | 3:CC:5:ILE:N       | 2.23                     | 0.53              |
| 4:CD:187:ARG:NH2   | 4:CD:193:ASP:OD2   | 2.41                     | 0.53              |
| 7:CG:120:ILE:HG22  | 7:CG:124:LEU:CD1   | 2.36                     | 0.53              |
| 11:CK:26:ASN:O     | 11:CK:27:ASN:HB2   | 2.06                     | 0.53              |
| 13:CM:11:ARG:HG2   | 13:CM:12:ASN:H     | 1.73                     | 0.53              |
| 20:CT:26:ASN:HB3   | 20:CT:71:THR:OG1   | 2.08                     | 0.53              |
| 24:CY:13:ARG:NH2   | 24:CY:282:SER:HB2  | 2.24                     | 0.53              |
| 24:CY:453:GLY:HA2  | 24:CY:458:HIS:HD2  | 1.72                     | 0.53              |
| 24:CY:84:THR:HG23  | 61:CY:702:FUA:H152 | 1.89                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:D2:14:ARG:HG3   | 27:D2:14:ARG:HH11  | 1.73                     | 0.53              |
| 31:D6:27:LYS:HZ2   | 31:D6:30:THR:CB    | 2.21                     | 0.53              |
| 35:DA:1713:U:O2'   | 35:DA:1714:G:H5'   | 2.08                     | 0.53              |
| 35:DA:1751:C:O2'   | 35:DA:1752:C:H5'   | 2.08                     | 0.53              |
| 35:DA:2030:A:H4'   | 35:DA:2031:A:H8    | 1.72                     | 0.53              |
| 35:DA:20:C:H2'     | 35:DA:21:A:H8      | 1.73                     | 0.53              |
| 35:DA:2206:G:C2    | 35:DA:2207:G:H5'   | 2.43                     | 0.53              |
| 35:DA:826:U:H5''   | 35:DA:2428:G:O3'   | 2.08                     | 0.53              |
| 34:D9:31:LYS:HE2   | 35:DA:2478:A:H5'   | 1.90                     | 0.53              |
| 35:DA:2749:A:N1    | 35:DA:2750:A:N6    | 2.57                     | 0.53              |
| 35:DA:569:U:C4     | 35:DA:570:G:C6     | 2.96                     | 0.53              |
| 35:DA:799:G:OP2    | 35:DA:800:A:H3'    | 2.09                     | 0.53              |
| 38:DD:183:ARG:HD2  | 38:DD:270:ILE:HG23 | 1.90                     | 0.53              |
| 35:DA:322:A:H3'    | 40:DF:169:ASN:ND2  | 2.23                     | 0.53              |
| 41:DG:41:GLN:O     | 41:DG:43:LEU:N     | 2.35                     | 0.53              |
| 44:DK:4:VAL:HG12   | 44:DK:5:VAL:N      | 2.20                     | 0.53              |
| 48:DP:16:ARG:O     | 48:DP:18:ARG:N     | 2.40                     | 0.53              |
| 48:DP:58:THR:O     | 48:DP:58:THR:HG22  | 2.09                     | 0.53              |
| 52:DT:60:THR:HG22  | 52:DT:77:PRO:HA    | 1.90                     | 0.53              |
| 57:DY:62:GLU:CG    | 57:DY:63:LYS:N     | 2.71                     | 0.53              |
| 58:DZ:56:VAL:HG22  | 58:DZ:91:LEU:CD1   | 2.38                     | 0.53              |
| 1:AA:1321:C:C5'    | 1:AA:1322:C:H5''   | 2.38                     | 0.53              |
| 1:AA:624:C:H4'     | 16:AP:10:GLY:C     | 2.29                     | 0.53              |
| 1:AA:818:G:O2'     | 1:AA:819:A:H5'     | 2.09                     | 0.53              |
| 4:AD:122:ARG:NH1   | 4:AD:134:ASP:HB2   | 2.23                     | 0.53              |
| 12:AL:23:LYS:HE3   | 12:AL:89:ARG:HE    | 1.73                     | 0.53              |
| 13:AM:81:LEU:HB3   | 13:AM:89:GLY:HA2   | 1.89                     | 0.53              |
| 18:AR:37:VAL:C     | 18:AR:39:VAL:H     | 2.11                     | 0.53              |
| 22:AW:53:G:H2'     | 22:AW:54:G:H8      | 1.74                     | 0.53              |
| 24:AY:238:THR:HG23 | 24:AY:240:GLU:H    | 1.73                     | 0.53              |
| 24:AY:486:THR:HG23 | 24:AY:600:VAL:CG1  | 2.38                     | 0.53              |
| 27:B2:41:ILE:CD1   | 27:B2:44:LEU:HD12  | 2.33                     | 0.53              |
| 31:B6:13:CYS:HB3   | 31:B6:49:HIS:HB3   | 1.90                     | 0.53              |
| 35:BA:1355:G:O2'   | 35:BA:1356:G:H5'   | 2.08                     | 0.53              |
| 35:BA:1791:A:C6    | 35:BA:1829:A:H5'   | 2.43                     | 0.53              |
| 35:BA:2012:G:H4'   | 55:BW:96:ILE:CD1   | 2.17                     | 0.53              |
| 35:BA:2346:A:H1'   | 35:BA:2383:G:N9    | 2.24                     | 0.53              |
| 35:BA:514:A:H2'    | 35:BA:515:A:H8     | 1.73                     | 0.53              |
| 35:BA:600:G:H2'    | 35:BA:601:C:C6     | 2.44                     | 0.53              |
| 35:BA:650:C:C3'    | 35:BA:651:G:H5''   | 2.38                     | 0.53              |
| 35:BA:848:G:H5''   | 35:BA:928:G:H22    | 1.72                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 37:BC:76:LEU:HD21 | 37:BC:104:ILE:HD11 | 1.91                     | 0.53              |
| 35:BA:1799:G:H8   | 38:BD:181:GLU:OE1  | 1.92                     | 0.53              |
| 38:BD:39:LYS:HZ2  | 38:BD:87:ASN:HB3   | 1.73                     | 0.53              |
| 39:BE:119:ARG:HD2 | 39:BE:120:TRP:NE1  | 2.24                     | 0.53              |
| 42:BH:84:SER:OG   | 42:BH:85:LYS:N     | 2.40                     | 0.53              |
| 46:BN:17:ASP:OD1  | 46:BN:56:ASN:HB3   | 2.08                     | 0.53              |
| 48:BP:25:SER:O    | 48:BP:30:THR:HG23  | 2.09                     | 0.53              |
| 51:BS:106:ARG:O   | 51:BS:107:GLU:CB   | 2.56                     | 0.53              |
| 52:BT:50:ILE:HA   | 52:BT:99:LEU:CD1   | 2.39                     | 0.53              |
| 54:BV:61:VAL:HG22 | 54:BV:63:GLY:H     | 1.74                     | 0.53              |
| 55:BW:12:ILE:HG13 | 55:BW:42:ARG:NH1   | 2.23                     | 0.53              |
| 56:BX:27:THR:CB   | 56:BX:80:ILE:HG22  | 2.36                     | 0.53              |
| 57:BY:15:VAL:O    | 57:BY:22:GLY:N     | 2.41                     | 0.53              |
| 57:BY:77:PRO:O    | 57:BY:78:ALA:HB2   | 2.08                     | 0.53              |
| 58:BZ:152:ALA:HB3 | 58:BZ:154:ASP:OD2  | 2.09                     | 0.53              |
| 1:CA:1004:A:H5'   | 1:CA:1025:U:N3     | 2.22                     | 0.53              |
| 1:CA:1118:C:H1'   | 1:CA:1179:A:C4     | 2.42                     | 0.53              |
| 2:CB:209:ARG:NH1  | 2:CB:239:VAL:HG11  | 2.23                     | 0.53              |
| 4:CD:192:GLU:O    | 4:CD:193:ASP:C     | 2.46                     | 0.53              |
| 6:CF:22:GLU:O     | 6:CF:26:ILE:HG13   | 2.07                     | 0.53              |
| 12:CL:70:ILE:CG2  | 12:CL:100:ILE:HD12 | 2.38                     | 0.53              |
| 13:CM:97:PRO:HA   | 13:CM:110:ARG:CD   | 2.33                     | 0.53              |
| 14:CN:37:PHE:CE1  | 14:CN:53:LEU:HD22  | 2.43                     | 0.53              |
| 24:CY:103:GLY:O   | 24:CY:104:ALA:CB   | 2.55                     | 0.53              |
| 24:CY:135:PHE:CD1 | 24:CY:272:LEU:HD22 | 2.42                     | 0.53              |
| 24:CY:439:ARG:O   | 24:CY:452:SER:HB3  | 2.08                     | 0.53              |
| 24:CY:483:TYR:O   | 24:CY:558:PHE:HB3  | 2.08                     | 0.53              |
| 27:D2:40:SER:C    | 27:D2:42:GLY:N     | 2.62                     | 0.53              |
| 29:D4:10:VAL:N    | 29:D4:26:SER:O     | 2.41                     | 0.53              |
| 33:D8:7:HIS:HB2   | 33:D8:59:LYS:HB3   | 1.89                     | 0.53              |
| 35:DA:221:A:H4'   | 35:DA:222:A:O5'    | 2.07                     | 0.53              |
| 35:DA:2347:C:H2'  | 35:DA:2348:U:C5    | 2.43                     | 0.53              |
| 35:DA:272(H):C:H6 | 35:DA:272(H):C:C5' | 2.17                     | 0.53              |
| 35:DA:359:A:H2'   | 35:DA:360:G:O4'    | 2.08                     | 0.53              |
| 35:DA:467:G:O2'   | 35:DA:468:G:H5'    | 2.09                     | 0.53              |
| 35:DA:492:A:H2'   | 35:DA:493:G:H5'    | 1.90                     | 0.53              |
| 35:DA:67:U:H2'    | 35:DA:68:G:C8      | 2.43                     | 0.53              |
| 28:D3:45:GLY:HA3  | 35:DA:851:U:O2'    | 2.08                     | 0.53              |
| 39:DE:2:LYS:HD3   | 39:DE:95:ILE:HG22  | 1.90                     | 0.53              |
| 46:DN:23:LEU:CB   | 46:DN:60:ILE:HG21  | 2.37                     | 0.53              |
| 46:DN:9:VAL:HG12  | 46:DN:10:GLU:N     | 2.23                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:DO:22:ILE:HG12  | 47:DO:41:ALA:HA    | 1.90                     | 0.53              |
| 51:DS:15:ARG:CB    | 51:DS:18:ILE:HD11  | 2.32                     | 0.53              |
| 51:DS:40:ILE:CG2   | 51:DS:41:ASP:N     | 2.72                     | 0.53              |
| 58:DZ:163:LEU:HD23 | 58:DZ:163:LEU:N    | 2.20                     | 0.53              |
| 1:AA:1258:G:H2'    | 1:AA:1259:C:C6     | 2.44                     | 0.53              |
| 1:AA:1324:A:H2'    | 1:AA:1325:C:H6     | 1.71                     | 0.53              |
| 1:AA:306:G:O2'     | 1:AA:307:C:H5'     | 2.08                     | 0.53              |
| 1:AA:998:G:H2'     | 1:AA:999:C:N1      | 2.24                     | 0.53              |
| 3:AC:59:ARG:HD3    | 3:AC:64:VAL:HG22   | 1.90                     | 0.53              |
| 5:AE:41:VAL:HG13   | 5:AE:113:ALA:HA    | 1.89                     | 0.53              |
| 6:AF:60:PHE:C      | 6:AF:61:LEU:HD12   | 2.28                     | 0.53              |
| 16:AP:2:VAL:O      | 16:AP:2:VAL:HG22   | 2.09                     | 0.53              |
| 18:AR:44:LEU:O     | 18:AR:45:SER:O     | 2.27                     | 0.53              |
| 20:AT:73:HIS:O     | 20:AT:74:LYS:C     | 2.47                     | 0.53              |
| 24:AY:186:TYR:HA   | 24:AY:198:GLU:HA   | 1.90                     | 0.53              |
| 24:AY:228:MET:O    | 24:AY:232:LEU:HD23 | 2.09                     | 0.53              |
| 26:B1:3:LYS:HE3    | 35:BA:1364:G:C8    | 2.43                     | 0.53              |
| 35:BA:1596:A:O2'   | 35:BA:1597:A:H5'   | 2.08                     | 0.53              |
| 35:BA:2861:G:H2'   | 35:BA:2862:G:H8    | 1.73                     | 0.53              |
| 35:BA:363(E):U:O2' | 35:BA:363(F):A:O4' | 2.26                     | 0.53              |
| 35:BA:852:G:H2'    | 35:BA:853:G:H8     | 1.73                     | 0.53              |
| 36:BB:68:C:O2'     | 36:BB:69:G:H5'     | 2.09                     | 0.53              |
| 40:BF:25:PRO:HB2   | 40:BF:119:ARG:HD3  | 1.89                     | 0.53              |
| 42:BH:149:ARG:HA   | 42:BH:162:ILE:HG13 | 1.91                     | 0.53              |
| 35:BA:558:G:H5'    | 46:BN:112:LEU:HD22 | 1.90                     | 0.53              |
| 46:BN:1:MET:HE2    | 46:BN:2:LYS:N      | 2.24                     | 0.53              |
| 48:BP:108:LYS:N    | 48:BP:108:LYS:HD2  | 2.23                     | 0.53              |
| 48:BP:112:LEU:H    | 48:BP:128:HIS:CD2  | 2.26                     | 0.53              |
| 49:BQ:62:GLY:HA2   | 58:BZ:116:VAL:CG2  | 2.38                     | 0.53              |
| 51:BS:89:ARG:NH1   | 51:BS:89:ARG:HG2   | 2.24                     | 0.53              |
| 52:BT:117:ASP:OD2  | 52:BT:120:ARG:HG3  | 2.08                     | 0.53              |
| 53:BU:49:HIS:C     | 53:BU:52:ARG:HB2   | 2.29                     | 0.53              |
| 58:BZ:86:VAL:HG12  | 58:BZ:87:ASP:N     | 2.19                     | 0.53              |
| 58:BZ:89:PHE:HE1   | 58:BZ:96:VAL:HG21  | 1.73                     | 0.53              |
| 1:CA:1329:A:O2'    | 1:CA:1330:U:H5'    | 2.09                     | 0.53              |
| 1:CA:265:G:H2'     | 1:CA:267:C:H5      | 1.73                     | 0.53              |
| 1:CA:275:G:H2'     | 1:CA:276:G:H8      | 1.73                     | 0.53              |
| 3:CC:154:SER:OG    | 3:CC:155:GLY:N     | 2.41                     | 0.53              |
| 4:CD:196:LEU:C     | 4:CD:198:VAL:H     | 2.12                     | 0.53              |
| 9:CI:69:GLY:O      | 9:CI:73:GLN:HG3    | 2.08                     | 0.53              |
| 10:CJ:20:ALA:C     | 10:CJ:22:LYS:N     | 2.61                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:CV:23:C:H2'     | 22:CV:24:U:H6      | 1.74                     | 0.53              |
| 22:CV:74:C:H2'     | 22:CV:75:C:H5'     | 1.90                     | 0.53              |
| 24:CY:18:ALA:O     | 24:CY:19:ALA:HB2   | 2.09                     | 0.53              |
| 24:CY:298:VAL:HG22 | 24:CY:299:VAL:N    | 2.23                     | 0.53              |
| 27:D2:4:SER:O      | 27:D2:6:VAL:N      | 2.42                     | 0.53              |
| 31:D6:15:GLU:OE1   | 31:D6:44:ARG:NH2   | 2.42                     | 0.53              |
| 31:D6:45:LYS:HG2   | 35:DA:2371:G:C5'   | 2.39                     | 0.53              |
| 35:DA:1052:C:H6    | 35:DA:1052:C:H3'   | 1.74                     | 0.53              |
| 35:DA:1107:G:OP1   | 43:DJ:58:UNK:HA    | 2.08                     | 0.53              |
| 35:DA:1173:G:H5'   | 35:DA:1174:A:O5'   | 2.08                     | 0.53              |
| 35:DA:1599:C:H2'   | 35:DA:1600:C:C6    | 2.41                     | 0.53              |
| 35:DA:1803:A:O3'   | 38:DD:259:THR:CG2  | 2.48                     | 0.53              |
| 35:DA:1887:C:C3'   | 35:DA:1888:G:H5''  | 2.38                     | 0.53              |
| 35:DA:2113:U:H2'   | 35:DA:2114:A:H8    | 1.73                     | 0.53              |
| 35:DA:2189:U:C3'   | 35:DA:2190:G:H5''  | 2.39                     | 0.53              |
| 26:D1:30:VAL:N     | 35:DA:2396:G:H4'   | 2.24                     | 0.53              |
| 35:DA:402:A:C2'    | 35:DA:403:U:H5'    | 2.39                     | 0.53              |
| 35:DA:503:A:H4'    | 35:DA:504:U:C5'    | 2.38                     | 0.53              |
| 35:DA:8:A:H2'      | 35:DA:9:U:C5       | 2.43                     | 0.53              |
| 35:DA:902:C:H2'    | 35:DA:903:C:C6     | 2.44                     | 0.53              |
| 38:DD:13:ARG:NH1   | 38:DD:16:MET:SD    | 2.82                     | 0.53              |
| 39:DE:34:VAL:HG11  | 39:DE:78:LEU:CD2   | 2.38                     | 0.53              |
| 41:DG:63:ILE:HG21  | 41:DG:141:PHE:CD2  | 2.44                     | 0.53              |
| 42:DH:44:VAL:HG12  | 42:DH:45:VAL:H     | 1.74                     | 0.53              |
| 42:DH:77:LYS:HA    | 42:DH:80:SER:OG    | 2.09                     | 0.53              |
| 45:DM:15:UNK:C     | 45:DM:17:UNK:N     | 3.29                     | 0.53              |
| 47:DO:60:ALA:C     | 47:DO:87:ILE:HD11  | 2.29                     | 0.53              |
| 48:DP:75:ILE:HD12  | 48:DP:75:ILE:N     | 2.23                     | 0.53              |
| 48:DP:85:LEU:CD2   | 48:DP:85:LEU:H     | 2.15                     | 0.53              |
| 56:DX:44:GLU:HB2   | 56:DX:49:VAL:O     | 2.08                     | 0.53              |
| 57:DY:38:ILE:HG23  | 57:DY:39:VAL:N     | 2.24                     | 0.53              |
| 57:DY:77:PRO:O     | 57:DY:78:ALA:HB2   | 2.09                     | 0.53              |
| 1:AA:10:A:H2'      | 1:AA:11:G:H8       | 1.73                     | 0.53              |
| 9:AI:104:ARG:O     | 9:AI:105:ASP:CB    | 2.57                     | 0.53              |
| 9:AI:84:ALA:C      | 9:AI:86:VAL:H      | 2.12                     | 0.53              |
| 10:AJ:3:LYS:HZ3    | 10:AJ:77:PRO:HD2   | 1.74                     | 0.53              |
| 10:AJ:51:ARG:H     | 10:AJ:60:ARG:HA    | 1.74                     | 0.53              |
| 22:AV:49:G:H1      | 22:AV:65:C:H42     | 1.55                     | 0.53              |
| 24:AY:411:VAL:HG12 | 24:AY:412:ALA:N    | 2.22                     | 0.53              |
| 24:AY:609:GLU:HB2  | 24:AY:670:VAL:HG22 | 1.91                     | 0.53              |
| 26:B1:76:ARG:HH22  | 26:B1:95:LEU:CG    | 2.21                     | 0.53              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 29:B4:22:ILE:N     | 29:B4:22:ILE:HD12 | 2.23                     | 0.53              |
| 31:B6:13:CYS:HA    | 31:B6:50:ARG:O    | 2.09                     | 0.53              |
| 35:BA:1141:U:H5'   | 46:BN:63:THR:CG2  | 2.39                     | 0.53              |
| 35:BA:2224:G:H4'   | 35:BA:2226:C:C2   | 2.43                     | 0.53              |
| 35:BA:284:U:H2'    | 35:BA:285:C:C6    | 2.43                     | 0.53              |
| 35:BA:402:A:C2'    | 35:BA:403:U:H5'   | 2.38                     | 0.53              |
| 35:BA:674:G:H2'    | 35:BA:804:A:H61   | 1.74                     | 0.53              |
| 35:BA:797:C:H2'    | 35:BA:798:G:H8    | 1.74                     | 0.53              |
| 38:BD:148:GLU:HB2  | 38:BD:151:LYS:CD  | 2.38                     | 0.53              |
| 38:BD:26:LYS:CA    | 38:BD:26:LYS:HE2  | 2.38                     | 0.53              |
| 39:BE:3:GLY:HA3    | 39:BE:81:ILE:HD12 | 1.90                     | 0.53              |
| 52:BT:64:ARG:HG2   | 52:BT:64:ARG:HH11 | 1.73                     | 0.53              |
| 1:CA:1030(D):A:C2' | 1:CA:1031:G:H5'   | 2.37                     | 0.53              |
| 1:CA:439:A:H2'     | 1:CA:441:A:H5'    | 1.91                     | 0.53              |
| 1:CA:867:G:O2'     | 1:CA:868:C:H5'    | 2.09                     | 0.53              |
| 2:CB:98:LEU:O      | 2:CB:101:MET:HB2  | 2.08                     | 0.53              |
| 3:CC:138:VAL:O     | 3:CC:139:GLN:C    | 2.47                     | 0.53              |
| 3:CC:95:THR:O      | 3:CC:97:LYS:N     | 2.41                     | 0.53              |
| 10:CJ:54:PHE:CD2   | 10:CJ:55:LYS:HE3  | 2.44                     | 0.53              |
| 15:CO:76:GLU:C     | 15:CO:78:TYR:N    | 2.61                     | 0.53              |
| 19:CS:41:VAL:O     | 19:CS:43:GLU:N    | 2.41                     | 0.53              |
| 24:CY:35:TYR:CE1   | 24:CY:269:VAL:HB  | 2.44                     | 0.53              |
| 24:CY:296:GLY:O    | 24:CY:297:GLU:CB  | 2.56                     | 0.53              |
| 28:D3:15:TYR:HD2   | 28:D3:19:GLN:HE22 | 1.54                     | 0.53              |
| 32:D7:24:THR:C     | 32:D7:26:GLY:H    | 2.11                     | 0.53              |
| 35:DA:1050:A:C5    | 35:DA:1051:G:H1'  | 2.44                     | 0.53              |
| 35:DA:1168:G:H2'   | 35:DA:1169:G:H8   | 1.74                     | 0.53              |
| 35:DA:1197:G:H2'   | 35:DA:1198:U:H6   | 1.72                     | 0.53              |
| 35:DA:2870:C:H2'   | 35:DA:2871:C:O4'  | 2.08                     | 0.53              |
| 35:DA:482:A:H4'    | 57:DY:47:LYS:HG2  | 1.90                     | 0.53              |
| 40:DF:154:VAL:HG11 | 40:DF:193:VAL:CG2 | 2.38                     | 0.53              |
| 40:DF:25:PRO:CB    | 40:DF:119:ARG:HD3 | 2.38                     | 0.53              |
| 58:DZ:168:GLU:O    | 58:DZ:169:GLU:C   | 2.47                     | 0.53              |
| 1:AA:275:G:H2'     | 1:AA:276:G:H8     | 1.74                     | 0.53              |
| 1:AA:631:G:C2'     | 1:AA:632:A:C8     | 2.92                     | 0.53              |
| 1:AA:865:A:H5'     | 1:AA:1078:U:O4    | 2.09                     | 0.53              |
| 1:AA:977:A:C2'     | 1:AA:978:A:H5'    | 2.39                     | 0.53              |
| 3:AC:77:ILE:HA     | 3:AC:84:ILE:HB    | 1.90                     | 0.53              |
| 4:AD:17:VAL:O      | 4:AD:18:LYS:O     | 2.26                     | 0.53              |
| 4:AD:187:ARG:NH2   | 4:AD:193:ASP:OD2  | 2.41                     | 0.53              |
| 6:AF:37:VAL:O      | 6:AF:38:GLU:HG3   | 2.08                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:AJ:54:PHE:CD2  | 10:AJ:55:LYS:HE3   | 2.44                     | 0.53              |
| 16:AP:25:ARG:NH1  | 16:AP:25:ARG:HG3   | 2.20                     | 0.53              |
| 19:AS:16:LEU:N    | 19:AS:16:LEU:HD12  | 2.24                     | 0.53              |
| 24:AY:164:MET:O   | 24:AY:165:GLN:HG2  | 2.09                     | 0.53              |
| 24:AY:177:ILE:O   | 24:AY:178:ILE:HD12 | 2.08                     | 0.53              |
| 24:AY:331:TYR:O   | 24:AY:371:ALA:HB1  | 2.08                     | 0.53              |
| 24:AY:684:GLN:O   | 24:AY:688:ILE:HD13 | 2.09                     | 0.53              |
| 25:B0:27:GLU:HG3  | 25:B0:68:GLU:HA    | 1.91                     | 0.53              |
| 27:B2:3:LEU:HD12  | 35:BA:98:G:H5''    | 1.90                     | 0.53              |
| 29:B4:16:CYS:SG   | 29:B4:17:GLY:N     | 2.81                     | 0.53              |
| 31:B6:42:TRP:CE3  | 31:B6:42:TRP:HA    | 2.44                     | 0.53              |
| 35:BA:1225:G:H2'  | 35:BA:1226:A:C8    | 2.43                     | 0.53              |
| 35:BA:1517:G:H5'  | 35:BA:1517:G:C8    | 2.37                     | 0.53              |
| 35:BA:2067:G:H1   | 35:BA:2443:C:H42   | 1.57                     | 0.53              |
| 35:BA:2688:U:H2'  | 35:BA:2719:G:N2    | 2.23                     | 0.53              |
| 35:BA:2750:A:H2'  | 35:BA:2752:C:N4    | 2.24                     | 0.53              |
| 35:BA:687:C:H2'   | 35:BA:688:U:O4'    | 2.09                     | 0.53              |
| 36:BB:68:C:H2'    | 36:BB:69:G:O4'     | 2.08                     | 0.53              |
| 38:BD:161:THR:O   | 38:BD:196:VAL:HG23 | 2.07                     | 0.53              |
| 41:BG:111:LEU:HA  | 41:BG:114:ILE:HD12 | 1.89                     | 0.53              |
| 47:BO:22:ILE:HG12 | 47:BO:41:ALA:HA    | 1.90                     | 0.53              |
| 54:BV:52:VAL:O    | 54:BV:52:VAL:HG13  | 2.08                     | 0.53              |
| 1:CA:1144:G:N2    | 1:CA:1146:A:H62    | 2.07                     | 0.53              |
| 1:CA:261:U:O2     | 1:CA:263:A:C8      | 2.62                     | 0.53              |
| 1:CA:936:C:O2'    | 1:CA:937:A:H5'     | 2.07                     | 0.53              |
| 3:CC:73:PRO:O     | 3:CC:76:VAL:HG22   | 2.09                     | 0.53              |
| 5:CE:135:THR:O    | 5:CE:138:ALA:HB3   | 2.07                     | 0.53              |
| 10:CJ:78:ASN:O    | 10:CJ:82:ILE:HG12  | 2.08                     | 0.53              |
| 24:CY:31:ARG:HD2  | 24:CY:266:ASN:OD1  | 2.08                     | 0.53              |
| 24:CY:512:ILE:N   | 24:CY:512:ILE:HD13 | 2.23                     | 0.53              |
| 24:CY:85:PRO:C    | 24:CY:87:HIS:H     | 2.11                     | 0.53              |
| 24:CY:85:PRO:HA   | 24:CY:94:VAL:HG13  | 1.91                     | 0.53              |
| 29:D4:19:GLY:O    | 29:D4:21:VAL:HG23  | 2.08                     | 0.53              |
| 35:DA:1568:G:OP2  | 38:DD:63:ARG:NH2   | 2.36                     | 0.53              |
| 35:DA:1635:G:H2'  | 35:DA:1636:C:C6    | 2.43                     | 0.53              |
| 35:DA:2026:C:N3   | 35:DA:2027:G:C8    | 2.77                     | 0.53              |
| 35:DA:2470:G:C6   | 35:DA:2471:C:C5    | 2.96                     | 0.53              |
| 35:DA:2820:A:O2'  | 35:DA:2821:A:OP1   | 2.25                     | 0.53              |
| 35:DA:281:G:N2    | 35:DA:358:U:C5     | 2.77                     | 0.53              |
| 35:DA:948:G:H1    | 35:DA:969:U:H3     | 1.57                     | 0.53              |
| 38:DD:108:PRO:HB3 | 38:DD:143:HIS:CE1  | 2.44                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:DD:112:GLN:H    | 38:DD:115:GLN:NE2  | 2.06                     | 0.53              |
| 40:DF:124:LEU:HD22 | 40:DF:191:ARG:HH21 | 1.72                     | 0.53              |
| 40:DF:127:GLU:HB2  | 40:DF:196:LEU:HD11 | 1.91                     | 0.53              |
| 44:DK:132:ARG:HH11 | 44:DK:132:ARG:HG3  | 1.72                     | 0.53              |
| 49:DQ:110:THR:HG22 | 49:DQ:113:GLN:OE1  | 2.09                     | 0.53              |
| 51:DS:25:ARG:HG3   | 51:DS:26:LEU:H     | 1.74                     | 0.53              |
| 51:DS:36:TYR:O     | 51:DS:37:ALA:HB2   | 2.07                     | 0.53              |
| 51:DS:70:GLY:C     | 51:DS:72:ALA:H     | 2.10                     | 0.53              |
| 58:DZ:20:ARG:HH11  | 58:DZ:20:ARG:CB    | 2.15                     | 0.53              |
| 1:AA:1307:U:H2'    | 1:AA:1308:U:C6     | 2.44                     | 0.53              |
| 1:AA:1378:C:O2     | 7:AG:76:ARG:NH2    | 2.42                     | 0.53              |
| 1:AA:164:U:H2'     | 1:AA:165:C:H6      | 1.73                     | 0.53              |
| 1:AA:353:A:H5'     | 1:AA:353:A:C8      | 2.41                     | 0.53              |
| 1:AA:407:G:H2'     | 1:AA:408:A:H8      | 1.73                     | 0.53              |
| 1:AA:538:G:O2'     | 1:AA:539:A:H5'     | 2.08                     | 0.53              |
| 6:AF:60:PHE:O      | 6:AF:61:LEU:HD12   | 2.08                     | 0.53              |
| 7:AG:146:GLU:HA    | 7:AG:149:ARG:HB2   | 1.90                     | 0.53              |
| 7:AG:38:LEU:O      | 7:AG:42:ILE:HG13   | 2.08                     | 0.53              |
| 7:AG:84:ASN:N      | 7:AG:84:ASN:HD22   | 2.07                     | 0.53              |
| 11:AK:20:TYR:HB2   | 11:AK:31:THR:HG22  | 1.91                     | 0.53              |
| 11:AK:26:ASN:O     | 11:AK:27:ASN:HB2   | 2.09                     | 0.53              |
| 12:AL:46:LYS:HB2   | 12:AL:92:ASP:O     | 2.09                     | 0.53              |
| 16:AP:20:VAL:HG23  | 16:AP:34:GLU:O     | 2.08                     | 0.53              |
| 18:AR:44:LEU:HD22  | 18:AR:79:LEU:HD22  | 1.91                     | 0.53              |
| 24:AY:606:MET:HE3  | 24:AY:671:MET:HG2  | 1.91                     | 0.53              |
| 25:B0:46:LYS:O     | 25:B0:78:TYR:HA    | 2.08                     | 0.53              |
| 31:B6:37:ARG:O     | 31:B6:48:VAL:O     | 2.26                     | 0.53              |
| 31:B6:5:VAL:CG1    | 31:B6:6:ARG:N      | 2.71                     | 0.53              |
| 31:B6:9:LEU:CD2    | 31:B6:26:ASN:HD22  | 2.21                     | 0.53              |
| 33:B8:29:LYS:HD2   | 33:B8:44:LYS:HG2   | 1.91                     | 0.53              |
| 35:BA:1052:C:H3'   | 35:BA:1052:C:H6    | 1.73                     | 0.53              |
| 35:BA:2647:U:H2'   | 35:BA:2648:C:H6    | 1.74                     | 0.53              |
| 35:BA:267:C:H2'    | 35:BA:268:C:C6     | 2.44                     | 0.53              |
| 35:BA:2681:C:H5    | 35:BA:2725:A:H62   | 1.57                     | 0.53              |
| 35:BA:271(H):G:H1  | 35:BA:271(P):C:H42 | 1.57                     | 0.53              |
| 35:BA:2888:C:H2'   | 35:BA:2889:C:H6    | 1.74                     | 0.53              |
| 35:BA:902:C:H2'    | 35:BA:903:C:C6     | 2.43                     | 0.53              |
| 38:BD:27:THR:O     | 38:BD:27:THR:HG23  | 2.07                     | 0.53              |
| 39:BE:55:ASN:O     | 39:BE:57:LYS:N     | 2.36                     | 0.53              |
| 40:BF:28:ILE:HG21  | 40:BF:116:ASP:HB2  | 1.90                     | 0.53              |
| 42:BH:68:THR:O     | 42:BH:70:THR:N     | 2.42                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:BK:74:ALA:HB2   | 44:BK:111:LYS:HE2  | 1.91                     | 0.53              |
| 46:BN:94:HIS:N     | 46:BN:95:PRO:CD    | 2.72                     | 0.53              |
| 47:BO:64:ARG:NE    | 52:BT:70:VAL:HG21  | 2.23                     | 0.53              |
| 35:BA:2394:C:P     | 48:BP:63:PRO:HD2   | 2.49                     | 0.53              |
| 54:BV:47:VAL:O     | 54:BV:49:THR:O     | 2.27                     | 0.53              |
| 55:BW:40:ASN:O     | 55:BW:41:LYS:HG2   | 2.09                     | 0.53              |
| 58:BZ:4:ARG:O      | 58:BZ:5:LEU:HB2    | 2.07                     | 0.53              |
| 1:CA:961:U:OP2     | 1:CA:1223:C:H4'    | 2.09                     | 0.53              |
| 1:CA:1239:A:C2'    | 1:CA:1298:C:N4     | 2.72                     | 0.53              |
| 1:CA:1442:G:C6     | 1:CA:1442(B):A:C2  | 2.90                     | 0.53              |
| 1:CA:375:U:H4'     | 16:CP:17:TYR:CE2   | 2.44                     | 0.53              |
| 2:CB:55:PHE:HA     | 2:CB:58:ILE:HD12   | 1.90                     | 0.53              |
| 4:CD:122:ARG:NH1   | 4:CD:134:ASP:HB2   | 2.24                     | 0.53              |
| 7:CG:43:PHE:O      | 7:CG:46:ALA:HB3    | 2.09                     | 0.53              |
| 8:CH:64:LYS:HD2    | 8:CH:79:VAL:HG21   | 1.91                     | 0.53              |
| 24:CY:14:ASN:ND2   | 24:CY:14:ASN:N     | 2.55                     | 0.53              |
| 24:CY:15:ILE:O     | 24:CY:15:ILE:HD12  | 2.08                     | 0.53              |
| 26:D1:18:ILE:HG21  | 26:D1:20:ARG:NE    | 2.23                     | 0.53              |
| 30:D5:3:LYS:HD2    | 30:D5:5:PRO:CD     | 2.37                     | 0.53              |
| 31:D6:15:GLU:HB2   | 31:D6:49:HIS:CE1   | 2.44                     | 0.53              |
| 34:D9:22:ARG:NH2   | 35:DA:2741:A:OP1   | 2.42                     | 0.53              |
| 35:DA:1097:U:H2'   | 35:DA:1098:A:H5'   | 1.91                     | 0.53              |
| 35:DA:1791:A:C6    | 35:DA:1829:A:H5'   | 2.44                     | 0.53              |
| 35:DA:1826:G:H4'   | 38:DD:242:ARG:NH2  | 2.15                     | 0.53              |
| 35:DA:2539:C:H2'   | 35:DA:2539:C:O2    | 2.09                     | 0.53              |
| 35:DA:2811:G:O2'   | 35:DA:2812:G:H5'   | 2.09                     | 0.53              |
| 35:DA:363(E):U:O2' | 35:DA:363(F):A:O4' | 2.27                     | 0.53              |
| 36:DB:16:G:N2      | 36:DB:69:G:H1'     | 2.24                     | 0.53              |
| 37:DC:88:GLU:HA    | 37:DC:95:VAL:HG21  | 1.91                     | 0.53              |
| 38:DD:142:VAL:HG23 | 38:DD:192:THR:C    | 2.29                     | 0.53              |
| 45:DL:65:UNK:O     | 45:DL:66:UNK:C     | 2.56                     | 0.53              |
| 48:DP:48:PRO:O     | 48:DP:50:ARG:N     | 2.42                     | 0.53              |
| 50:DR:9:LYS:O      | 50:DR:10:LEU:CD2   | 2.57                     | 0.53              |
| 51:DS:17:ARG:HA    | 51:DS:20:ARG:NH1   | 2.24                     | 0.53              |
| 58:DZ:109:ALA:HB3  | 58:DZ:145:GLU:HA   | 1.90                     | 0.53              |
| 1:AA:1113:C:H2'    | 1:AA:1114:C:H6     | 1.73                     | 0.53              |
| 1:AA:796:C:O2      | 1:AA:796:C:H2'     | 2.08                     | 0.53              |
| 2:AB:51:LEU:HD21   | 2:AB:201:ILE:HG23  | 1.91                     | 0.53              |
| 2:AB:55:PHE:HA     | 2:AB:58:ILE:HD12   | 1.89                     | 0.53              |
| 4:AD:132:ARG:HD2   | 4:AD:132:ARG:O     | 2.08                     | 0.53              |
| 5:AE:10:MET:HG3    | 5:AE:32:VAL:HG22   | 1.91                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:AE:11:ILE:HG13  | 5:AE:33:VAL:HG23   | 1.91                     | 0.53              |
| 12:AL:6:THR:OG1   | 12:AL:9:GLN:HG3    | 2.09                     | 0.53              |
| 16:AP:75:ARG:O    | 16:AP:78:GLY:N     | 2.41                     | 0.53              |
| 13:AM:94:ARG:NE   | 19:AS:82:GLY:N     | 2.57                     | 0.53              |
| 22:AW:69:C:O2'    | 22:AW:70:C:O4'     | 2.22                     | 0.53              |
| 24:AY:607:ARG:O   | 24:AY:671:MET:HA   | 2.09                     | 0.53              |
| 33:B8:7:HIS:HB2   | 33:B8:59:LYS:HB3   | 1.89                     | 0.53              |
| 35:BA:1291:C:H2'  | 35:BA:1292:U:C6    | 2.44                     | 0.53              |
| 35:BA:1441:G:H2'  | 35:BA:1442:G:C8    | 2.43                     | 0.53              |
| 35:BA:1858:G:HO2' | 35:BA:1859:A:H8    | 1.55                     | 0.53              |
| 35:BA:569:U:C4    | 35:BA:570:G:C6     | 2.97                     | 0.53              |
| 35:BA:665:C:H2'   | 35:BA:666:G:H8     | 1.74                     | 0.53              |
| 35:BA:84:A:C5'    | 57:BY:9:LYS:HZ2    | 2.19                     | 0.53              |
| 36:BB:94:C:H2'    | 36:BB:95:C:C6      | 2.44                     | 0.53              |
| 38:BD:125:ILE:O   | 38:BD:125:ILE:HG22 | 2.09                     | 0.53              |
| 35:BA:2679:A:H4'  | 39:BE:165:VAL:HG11 | 1.90                     | 0.53              |
| 39:BE:2:LYS:HD3   | 39:BE:95:ILE:HG22  | 1.91                     | 0.53              |
| 40:BF:50:SER:HB2  | 40:BF:94:PRO:HD3   | 1.90                     | 0.53              |
| 40:BF:7:TYR:OH    | 40:BF:10:PRO:HG3   | 2.09                     | 0.53              |
| 42:BH:127:GLU:HB3 | 42:BH:128:PRO:HD2  | 1.91                     | 0.53              |
| 42:BH:97:ARG:O    | 42:BH:98:LEU:C     | 2.48                     | 0.53              |
| 35:BA:1276:A:H1'  | 50:BR:16:HIS:HE1   | 1.74                     | 0.53              |
| 53:BU:12:ARG:HB3  | 53:BU:16:LYS:HE3   | 1.91                     | 0.53              |
| 1:CA:1115:C:H2'   | 1:CA:1116:C:H6     | 1.74                     | 0.53              |
| 1:CA:1300:G:O2'   | 1:CA:1301:U:P      | 2.67                     | 0.53              |
| 1:CA:1510:U:H2'   | 1:CA:1511:G:C8     | 2.43                     | 0.53              |
| 1:CA:624:C:O2'    | 1:CA:625:G:H5'     | 2.09                     | 0.53              |
| 2:CB:207:ALA:O    | 2:CB:211:ILE:HG13  | 2.09                     | 0.53              |
| 4:CD:126:ILE:CG2  | 4:CD:127:THR:N     | 2.71                     | 0.53              |
| 4:CD:107:ARG:HH21 | 4:CD:194:LEU:HD12  | 1.74                     | 0.53              |
| 5:CE:64:ARG:NH1   | 5:CE:64:ARG:CG     | 2.71                     | 0.53              |
| 9:CI:3:GLN:NE2    | 9:CI:20:ARG:NH2    | 2.56                     | 0.53              |
| 15:CO:11:VAL:O    | 15:CO:12:ILE:C     | 2.48                     | 0.53              |
| 20:CT:42:GLN:NE2  | 20:CT:42:GLN:HA    | 2.24                     | 0.53              |
| 25:D0:46:LYS:O    | 25:D0:78:TYR:HA    | 2.08                     | 0.53              |
| 26:D1:52:ARG:NH1  | 35:DA:2218:U:O2'   | 2.42                     | 0.53              |
| 28:D3:31:LEU:O    | 28:D3:32:GLN:HB2   | 2.09                     | 0.53              |
| 31:D6:10:LEU:HD12 | 33:D8:34:TRP:HB2   | 1.89                     | 0.53              |
| 31:D6:31:PRO:O    | 31:D6:32:ASN:OD1   | 2.27                     | 0.53              |
| 33:D8:13:ARG:HB3  | 48:DP:63:PRO:HB3   | 1.90                     | 0.53              |
| 35:DA:1047:G:HO2' | 35:DA:1110:G:N2    | 2.07                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:1102:C:H2'   | 35:DA:1103:A:H8    | 1.73                     | 0.53              |
| 35:DA:1336:A:H2'   | 35:DA:1337:G:H8    | 1.74                     | 0.53              |
| 35:DA:1819:A:H1'   | 35:DA:1821:A:C6    | 2.44                     | 0.53              |
| 35:DA:1821:A:H2'   | 35:DA:1822:G:H8    | 1.74                     | 0.53              |
| 35:DA:2051:A:H4'   | 39:DE:141:ILE:HD13 | 1.91                     | 0.53              |
| 35:DA:271(H):G:H1  | 35:DA:271(P):C:H42 | 1.56                     | 0.53              |
| 35:DA:272(I):U:C4  | 35:DA:363(A):A:N1  | 2.75                     | 0.53              |
| 35:DA:705:A:N1     | 35:DA:727:A:H1'    | 2.23                     | 0.53              |
| 38:DD:148:GLU:HB2  | 38:DD:151:LYS:CD   | 2.38                     | 0.53              |
| 35:DA:729:G:N7     | 38:DD:208:LYS:HB2  | 2.24                     | 0.53              |
| 41:DG:111:LEU:HA   | 41:DG:114:ILE:CD1  | 2.38                     | 0.53              |
| 41:DG:133:LEU:O    | 41:DG:157:ILE:HB   | 2.09                     | 0.53              |
| 41:DG:181:ARG:HG3  | 41:DG:181:ARG:HH11 | 1.74                     | 0.53              |
| 41:DG:41:GLN:C     | 41:DG:43:LEU:H     | 2.10                     | 0.53              |
| 42:DH:144:VAL:O    | 42:DH:148:ILE:HG12 | 2.08                     | 0.53              |
| 42:DH:159:GLU:O    | 42:DH:160:LYS:O    | 2.26                     | 0.53              |
| 45:DL:80:UNK:O     | 45:DL:82:UNK:N     | 2.42                     | 0.53              |
| 46:DN:17:ASP:OD1   | 46:DN:56:ASN:HB3   | 2.08                     | 0.53              |
| 49:DQ:135:ASP:O    | 49:DQ:138:ASP:OD2  | 2.27                     | 0.53              |
| 53:DU:104:GLN:HB3  | 54:DV:44:LYS:NZ    | 2.24                     | 0.53              |
| 54:DV:47:VAL:O     | 54:DV:49:THR:O     | 2.26                     | 0.53              |
| 57:DY:86:ARG:H     | 57:DY:88:LYS:NZ    | 2.07                     | 0.53              |
| 58:DZ:17:ALA:HA    | 58:DZ:20:ARG:CG    | 2.38                     | 0.53              |
| 1:AA:1356:G:H2'    | 1:AA:1357:A:H8     | 1.69                     | 0.53              |
| 1:AA:268:C:O2      | 1:AA:268:C:H2'     | 2.08                     | 0.53              |
| 1:AA:554:C:H2'     | 1:AA:555:C:C6      | 2.44                     | 0.53              |
| 1:AA:812:C:O2'     | 1:AA:813:U:P       | 2.67                     | 0.53              |
| 3:AC:164:ARG:NH2   | 3:AC:166:GLU:OE1   | 2.42                     | 0.53              |
| 6:AF:67:MET:HB2    | 6:AF:68:PRO:CD     | 2.37                     | 0.53              |
| 12:AL:110:VAL:HG21 | 12:AL:120:TYR:HD2  | 1.74                     | 0.53              |
| 16:AP:9:PHE:CE2    | 16:AP:18:ARG:CZ    | 2.92                     | 0.53              |
| 22:AV:35:A:O2'     | 22:AV:36:U:H5'     | 2.09                     | 0.53              |
| 24:AY:113:GLY:O    | 24:AY:115:GLU:N    | 2.42                     | 0.53              |
| 24:AY:28:THR:O     | 24:AY:32:ILE:HG13  | 2.09                     | 0.53              |
| 24:AY:446:THR:O    | 24:AY:448:GLN:N    | 2.41                     | 0.53              |
| 24:AY:584:ILE:O    | 24:AY:588:MET:HG3  | 2.09                     | 0.53              |
| 24:AY:90:PHE:O     | 24:AY:90:PHE:CG    | 2.62                     | 0.53              |
| 31:B6:15:GLU:C     | 31:B6:16:CYS:O     | 2.45                     | 0.53              |
| 31:B6:15:GLU:CD    | 31:B6:44:ARG:CZ    | 2.77                     | 0.53              |
| 31:B6:45:LYS:HG2   | 35:BA:2371:G:C5'   | 2.39                     | 0.53              |
| 35:BA:1233:C:H2'   | 35:BA:1234:U:H6    | 1.74                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:1432:C:H2'   | 35:BA:1433:U:O4'   | 2.09                     | 0.53              |
| 35:BA:272(I):U:H5  | 35:BA:363(A):A:H2  | 1.57                     | 0.53              |
| 35:BA:2839:G:H2'   | 35:BA:2840:C:C6    | 2.44                     | 0.53              |
| 35:BA:493:G:H2'    | 35:BA:494:G:O4'    | 2.09                     | 0.53              |
| 35:BA:503:A:H4'    | 35:BA:504:U:H5'    | 1.91                     | 0.53              |
| 35:BA:860:U:H5     | 35:BA:917:A:N7     | 2.07                     | 0.53              |
| 37:BC:28:ARG:HH12  | 37:BC:183:PRO:HB2  | 1.74                     | 0.53              |
| 46:BN:23:LEU:CB    | 46:BN:60:ILE:HG21  | 2.39                     | 0.53              |
| 48:BP:47:ASP:OD1   | 48:BP:49:ARG:HB2   | 2.09                     | 0.53              |
| 50:BR:113:LEU:HD12 | 50:BR:114:VAL:H    | 1.73                     | 0.53              |
| 35:BA:495:G:H1'    | 55:BW:57:ASN:OD1   | 2.08                     | 0.53              |
| 58:BZ:111:VAL:O    | 58:BZ:112:ARG:HB2  | 2.07                     | 0.53              |
| 1:CA:1030:C:H2'    | 1:CA:1030(A):G:H5' | 1.91                     | 0.53              |
| 1:CA:1271:G:H2'    | 1:CA:1272:G:C8     | 2.44                     | 0.53              |
| 1:CA:1368:G:C2'    | 1:CA:1369:C:H5'    | 2.39                     | 0.53              |
| 1:CA:793:U:O2      | 1:CA:1516:G:H4'    | 2.09                     | 0.53              |
| 1:CA:192:U:H2'     | 1:CA:193:C:H6      | 1.74                     | 0.53              |
| 1:CA:284:G:H2'     | 1:CA:285:G:H8      | 1.74                     | 0.53              |
| 1:CA:39:G:O2'      | 1:CA:40:C:H5'      | 2.08                     | 0.53              |
| 1:CA:707:C:O2'     | 1:CA:708:C:H5'     | 2.08                     | 0.53              |
| 1:CA:972:C:H4'     | 10:CJ:57:LYS:HB2   | 1.91                     | 0.53              |
| 3:CC:23:TYR:CG     | 3:CC:24:ALA:N      | 2.77                     | 0.53              |
| 4:CD:33:MET:HG3    | 4:CD:37:PRO:HA     | 1.90                     | 0.53              |
| 6:CF:21:LEU:O      | 6:CF:25:ILE:HG12   | 2.09                     | 0.53              |
| 7:CG:18:TYR:CD2    | 7:CG:59:LEU:HD13   | 2.44                     | 0.53              |
| 13:CM:52:GLU:HA    | 13:CM:55:ARG:HD3   | 1.91                     | 0.53              |
| 1:CA:1202:G:C2     | 14:CN:42:ILE:HG21  | 2.44                     | 0.53              |
| 17:CQ:12:SER:HB3   | 17:CQ:20:THR:OG1   | 2.09                     | 0.53              |
| 18:CR:37:VAL:HG23  | 18:CR:38:GLU:HG2   | 1.90                     | 0.53              |
| 20:CT:88:VAL:O     | 20:CT:92:LEU:HG    | 2.09                     | 0.53              |
| 24:CY:440:VAL:HG12 | 24:CY:449:THR:HG21 | 1.91                     | 0.53              |
| 24:CY:590:ILE:HD13 | 24:CY:593:ALA:CB   | 2.39                     | 0.53              |
| 30:D5:27:PRO:CD    | 55:DW:23:LEU:HD11  | 2.39                     | 0.53              |
| 31:D6:16:CYS:O     | 31:D6:17:LYS:HB2   | 2.08                     | 0.53              |
| 35:DA:1156:A:C2'   | 35:DA:1157:G:OP1   | 2.57                     | 0.53              |
| 35:DA:1230:C:H2'   | 35:DA:1231:G:C8    | 2.44                     | 0.53              |
| 35:DA:1759:A:H5'   | 35:DA:2715:C:H1'   | 1.90                     | 0.53              |
| 35:DA:2156:G:H2'   | 35:DA:2157:G:O4'   | 2.09                     | 0.53              |
| 35:DA:267:C:H2'    | 35:DA:268:C:C6     | 2.44                     | 0.53              |
| 35:DA:2732:G:H3'   | 35:DA:2733:A:C5'   | 2.37                     | 0.53              |
| 35:DA:536:A:H2'    | 35:DA:537:C:C6     | 2.43                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:572:A:C2     | 35:DA:2033:A:C2    | 2.97                     | 0.53              |
| 35:DA:852:G:H2'    | 35:DA:853:G:H8     | 1.74                     | 0.53              |
| 37:DC:92:ALA:HB3   | 37:DC:95:VAL:HG22  | 1.90                     | 0.53              |
| 38:DD:35:LYS:HZ2   | 38:DD:35:LYS:HB3   | 1.74                     | 0.53              |
| 39:DE:3:GLY:HA3    | 39:DE:81:ILE:HD12  | 1.91                     | 0.53              |
| 42:DH:13:LYS:O     | 42:DH:15:VAL:N     | 2.37                     | 0.53              |
| 44:DK:84:LEU:HD21  | 44:DK:96:VAL:HB    | 1.91                     | 0.53              |
| 47:DO:111:PHE:O    | 47:DO:115:VAL:HG23 | 2.09                     | 0.53              |
| 35:DA:1161:C:H1'   | 54:DV:8:GLY:O      | 2.09                     | 0.53              |
| 57:DY:99:CYS:O     | 57:DY:100:ALA:O    | 2.27                     | 0.53              |
| 1:AA:1030(D):A:C2' | 1:AA:1031:G:H5'    | 2.38                     | 0.52              |
| 1:AA:1490:C:C6     | 1:AA:1490:C:C5'    | 2.88                     | 0.52              |
| 2:AB:115:LEU:HD13  | 2:AB:145:LEU:HB3   | 1.91                     | 0.52              |
| 3:AC:131:ARG:NH2   | 3:AC:168:ALA:HB2   | 2.24                     | 0.52              |
| 3:AC:72:LYS:HA     | 3:AC:72:LYS:HE3    | 1.90                     | 0.52              |
| 4:AD:33:MET:HG3    | 4:AD:37:PRO:HA     | 1.90                     | 0.52              |
| 6:AF:22:GLU:O      | 6:AF:26:ILE:HG13   | 2.09                     | 0.52              |
| 6:AF:24:GLU:OE2    | 6:AF:28:ARG:NH1    | 2.42                     | 0.52              |
| 6:AF:80:ARG:NH1    | 6:AF:88:VAL:HB     | 2.23                     | 0.52              |
| 17:AQ:12:SER:HB3   | 17:AQ:20:THR:OG1   | 2.09                     | 0.52              |
| 19:AS:41:VAL:O     | 19:AS:43:GLU:N     | 2.42                     | 0.52              |
| 13:AM:91:ARG:HH21  | 19:AS:81:ARG:HH21  | 1.57                     | 0.52              |
| 22:AW:20:G:C5      | 35:BA:2169:A:C2    | 2.97                     | 0.52              |
| 22:AW:2:G:H2'      | 22:AW:3:C:C6       | 2.45                     | 0.52              |
| 24:AY:312:LEU:HD11 | 24:AY:401:SER:OG   | 2.09                     | 0.52              |
| 35:BA:134:C:H2'    | 35:BA:135:G:C8     | 2.43                     | 0.52              |
| 35:BA:2113:U:H2'   | 35:BA:2114:A:H8    | 1.74                     | 0.52              |
| 35:BA:212:G:C8     | 35:BA:212:G:H5'    | 2.34                     | 0.52              |
| 35:BA:358:U:H2'    | 35:BA:359:A:C8     | 2.28                     | 0.52              |
| 35:BA:654(P):C:H2' | 35:BA:654(Q):C:H5' | 1.91                     | 0.52              |
| 35:BA:784:A:HO2'   | 35:BA:785:G:H8     | 1.55                     | 0.52              |
| 35:BA:813:U:H2'    | 35:BA:814:C:C5     | 2.44                     | 0.52              |
| 37:BC:88:GLU:HA    | 37:BC:95:VAL:HG21  | 1.91                     | 0.52              |
| 38:BD:118:VAL:HG22 | 38:BD:119:ALA:N    | 2.24                     | 0.52              |
| 35:BA:729:G:N7     | 38:BD:208:LYS:HB2  | 2.24                     | 0.52              |
| 40:BF:25:PRO:CB    | 40:BF:119:ARG:HD3  | 2.39                     | 0.52              |
| 42:BH:72:ILE:O     | 42:BH:75:ALA:N     | 2.41                     | 0.52              |
| 44:BK:112:MET:N    | 44:BK:113:PRO:CD   | 2.72                     | 0.52              |
| 46:BN:3:THR:C      | 46:BN:4:TYR:CG     | 2.81                     | 0.52              |
| 51:BS:103:GLU:O    | 51:BS:104:GLY:C    | 2.47                     | 0.52              |
| 55:BW:20:VAL:HG23  | 55:BW:21:VAL:N     | 2.24                     | 0.52              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1131:G:C6    | 1:CA:1132:C:N4     | 2.78                     | 0.52              |
| 1:CA:1226:C:H5'   | 13:CM:96:LEU:CD1   | 2.38                     | 0.52              |
| 1:CA:1342:C:H1'   | 9:CI:124:GLN:HG3   | 1.90                     | 0.52              |
| 1:CA:937:A:C2     | 1:CA:1379:G:O6     | 2.62                     | 0.52              |
| 1:CA:189(A):C:H2' | 1:CA:189(B):C:H6   | 1.72                     | 0.52              |
| 1:CA:708:C:H2'    | 1:CA:709:G:H8      | 1.75                     | 0.52              |
| 2:CB:194:PRO:O    | 2:CB:196:LEU:N     | 2.42                     | 0.52              |
| 2:CB:86:GLU:C     | 2:CB:88:ALA:H      | 2.11                     | 0.52              |
| 7:CG:29:LYS:CB    | 7:CG:105:VAL:HG21  | 2.39                     | 0.52              |
| 7:CG:91:VAL:HG12  | 7:CG:92:SER:H      | 1.74                     | 0.52              |
| 8:CH:114:THR:HG21 | 8:CH:129:VAL:HG23  | 1.91                     | 0.52              |
| 9:CI:48:GLU:N     | 9:CI:49:PRO:CD     | 2.72                     | 0.52              |
| 10:CJ:6:ILE:HG13  | 10:CJ:72:VAL:O     | 2.09                     | 0.52              |
| 12:CL:46:LYS:HZ2  | 12:CL:94:PRO:HG3   | 1.74                     | 0.52              |
| 15:CO:43:LEU:HD12 | 15:CO:56:LEU:HD22  | 1.92                     | 0.52              |
| 16:CP:7:ALA:O     | 16:CP:17:TYR:HA    | 2.09                     | 0.52              |
| 18:CR:44:LEU:HD22 | 18:CR:79:LEU:HD22  | 1.90                     | 0.52              |
| 19:CS:43:GLU:O    | 19:CS:45:VAL:HG13  | 2.09                     | 0.52              |
| 22:CW:2:G:H2'     | 22:CW:3:C:H6       | 1.73                     | 0.52              |
| 24:CY:247:ARG:O   | 24:CY:251:ILE:HG13 | 2.09                     | 0.52              |
| 24:CY:496:LYS:HE2 | 24:CY:498:ILE:CD1  | 2.39                     | 0.52              |
| 24:CY:609:GLU:HB2 | 24:CY:670:VAL:HG22 | 1.91                     | 0.52              |
| 24:CY:625:ASN:C   | 24:CY:627:ARG:H    | 2.12                     | 0.52              |
| 30:D5:40:LYS:HZ1  | 30:D5:46:CYS:H     | 1.56                     | 0.52              |
| 31:D6:5:VAL:CG1   | 31:D6:6:ARG:N      | 2.72                     | 0.52              |
| 31:D6:8:LYS:HE3   | 31:D6:25:LYS:CD    | 2.31                     | 0.52              |
| 35:DA:1035:U:H2'  | 35:DA:1036:G:H8    | 1.72                     | 0.52              |
| 35:DA:2205:C:O2   | 35:DA:2205:C:H2'   | 2.08                     | 0.52              |
| 35:DA:2373:G:H2'  | 35:DA:2374:C:C6    | 2.44                     | 0.52              |
| 36:DB:13:A:O2'    | 36:DB:15:A:H5''    | 2.09                     | 0.52              |
| 39:DE:105:THR:OG1 | 39:DE:199:ARG:NH2  | 2.41                     | 0.52              |
| 40:DF:9:ILE:HG12  | 40:DF:14:PRO:C     | 2.28                     | 0.52              |
| 41:DG:123:ASN:O   | 41:DG:125:PHE:N    | 2.41                     | 0.52              |
| 42:DH:88:LEU:HD23 | 42:DH:164:TYR:O    | 2.09                     | 0.52              |
| 48:DP:102:ARG:CB  | 48:DP:102:ARG:NH2  | 2.70                     | 0.52              |
| 49:DQ:55:VAL:HG23 | 58:DZ:178:GLU:CG   | 2.39                     | 0.52              |
| 50:DR:4:LEU:C     | 50:DR:6:SER:H      | 2.12                     | 0.52              |
| 51:DS:103:GLU:O   | 51:DS:104:GLY:C    | 2.47                     | 0.52              |
| 53:DU:62:ILE:HG23 | 53:DU:76:TYR:CE1   | 2.44                     | 0.52              |
| 1:AA:1073:U:O2'   | 1:AA:1074:G:H5'    | 2.09                     | 0.52              |
| 1:AA:444:C:H42    | 1:AA:490:G:H1      | 1.57                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:AB:62:ALA:O      | 2:AB:64:ARG:N      | 2.34                     | 0.52              |
| 3:AC:59:ARG:CG     | 3:AC:64:VAL:HA     | 2.39                     | 0.52              |
| 6:AF:42:GLU:C      | 6:AF:44:GLY:H      | 2.12                     | 0.52              |
| 12:AL:84:LEU:HD23  | 12:AL:101:VAL:HG21 | 1.91                     | 0.52              |
| 24:AY:165:GLN:NE2  | 24:AY:177:ILE:HG21 | 2.25                     | 0.52              |
| 24:AY:181:LEU:CD1  | 24:AY:242:LEU:HD13 | 2.40                     | 0.52              |
| 24:AY:196:ILE:O    | 24:AY:197:ARG:CB   | 2.56                     | 0.52              |
| 24:AY:423:LYS:CB   | 24:AY:472:VAL:HG22 | 2.28                     | 0.52              |
| 24:AY:89:ASP:OD2   | 24:AY:89:ASP:N     | 2.43                     | 0.52              |
| 28:B3:31:LEU:HD22  | 28:B3:32:GLN:N     | 2.24                     | 0.52              |
| 30:B5:46:CYS:SG    | 30:B5:47:PRO:HD2   | 2.50                     | 0.52              |
| 33:B8:7:HIS:HB3    | 33:B8:10:ALA:HB3   | 1.91                     | 0.52              |
| 35:BA:2105:C:C2'   | 35:BA:2106:G:H5'   | 2.39                     | 0.52              |
| 35:BA:234:C:H2'    | 35:BA:235:U:C6     | 2.44                     | 0.52              |
| 35:BA:2389:G:H5''  | 35:BA:2390:U:C5'   | 2.36                     | 0.52              |
| 35:BA:2787:C:C2    | 39:BE:61:ARG:HD3   | 2.44                     | 0.52              |
| 35:BA:816:C:O2'    | 35:BA:817:C:H5'    | 2.08                     | 0.52              |
| 35:BA:675:A:H4'    | 40:BF:67:GLN:OE1   | 2.10                     | 0.52              |
| 44:BK:112:MET:HE1  | 44:BK:120:LEU:HD21 | 1.92                     | 0.52              |
| 45:BM:26:UNK:HA    | 45:BM:30:UNK:O     | 2.10                     | 0.52              |
| 46:BN:18:ALA:HB3   | 46:BN:21:LYS:HB2   | 1.92                     | 0.52              |
| 47:BO:104:ARG:NH2  | 52:BT:33:LYS:HE3   | 2.24                     | 0.52              |
| 48:BP:127:ALA:HB3  | 48:BP:130:PHE:CE1  | 2.44                     | 0.52              |
| 49:BQ:58:PHE:O     | 49:BQ:58:PHE:HD1   | 1.92                     | 0.52              |
| 50:BR:72:ASP:CG    | 50:BR:75:LEU:H     | 2.12                     | 0.52              |
| 51:BS:26:LEU:O     | 51:BS:88:ASP:HB3   | 2.09                     | 0.52              |
| 54:BV:39:LEU:HD22  | 54:BV:39:LEU:N     | 2.24                     | 0.52              |
| 57:BY:74:PRO:O     | 57:BY:75:ILE:HB    | 2.09                     | 0.52              |
| 1:CA:1053:G:H4'    | 1:CA:1054:C:H5'    | 1.90                     | 0.52              |
| 1:CA:1271:G:H2'    | 1:CA:1272:G:H8     | 1.74                     | 0.52              |
| 1:CA:129(A):G:C8   | 1:CA:129(A):G:H5'' | 2.45                     | 0.52              |
| 1:CA:328:C:C2'     | 1:CA:328:C:O2      | 2.56                     | 0.52              |
| 1:CA:424:G:H2'     | 1:CA:425:G:H8      | 1.75                     | 0.52              |
| 7:CG:12:LEU:CD1    | 7:CG:25:ALA:HB2    | 2.39                     | 0.52              |
| 20:CT:48:LYS:HD2   | 20:CT:51:GLU:OE2   | 2.08                     | 0.52              |
| 24:CY:510:VAL:HG22 | 24:CY:534:ILE:HD11 | 1.91                     | 0.52              |
| 24:CY:409:ILE:CD1  | 24:CY:654:GLY:HA2  | 2.39                     | 0.52              |
| 24:CY:138:LYS:HG2  | 62:CY:703:GDP:C5   | 2.44                     | 0.52              |
| 29:D4:31:ILE:CG2   | 29:D4:33:VAL:HG23  | 2.39                     | 0.52              |
| 33:D8:15:LYS:HB2   | 48:DP:65:ARG:HH12  | 1.73                     | 0.52              |
| 35:DA:1398:C:H2'   | 35:DA:1399:C:H6    | 1.72                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:DB:60:C:H2'     | 36:DB:61:G:C8      | 2.41                     | 0.52              |
| 37:DC:88:GLU:CA    | 37:DC:95:VAL:HG21  | 2.40                     | 0.52              |
| 38:DD:238:GLY:O    | 38:DD:239:ARG:O    | 2.27                     | 0.52              |
| 41:DG:159:VAL:O    | 41:DG:159:VAL:HG22 | 2.10                     | 0.52              |
| 41:DG:82:LEU:HD13  | 41:DG:87:PRO:HB3   | 1.90                     | 0.52              |
| 46:DN:14:VAL:HG13  | 46:DN:137:LYS:HG3  | 1.90                     | 0.52              |
| 48:DP:107:LYS:C    | 48:DP:109:GLY:H    | 2.12                     | 0.52              |
| 35:DA:637:A:OP2    | 48:DP:115:LEU:HB2  | 2.09                     | 0.52              |
| 48:DP:83:VAL:HG11  | 48:DP:112:LEU:HD21 | 1.90                     | 0.52              |
| 30:D5:44:THR:HG23  | 50:DR:101:ALA:N    | 2.25                     | 0.52              |
| 50:DR:55:ALA:HB2   | 50:DR:79:LEU:HD11  | 1.92                     | 0.52              |
| 52:DT:120:ARG:HA   | 52:DT:123:GLN:HG2  | 1.91                     | 0.52              |
| 52:DT:62:THR:HG22  | 52:DT:75:ILE:HG13  | 1.90                     | 0.52              |
| 57:DY:84:ARG:NH1   | 57:DY:84:ARG:HG2   | 2.22                     | 0.52              |
| 58:DZ:94:GLU:O     | 58:DZ:130:PRO:HD3  | 2.09                     | 0.52              |
| 58:DZ:72:ARG:HG3   | 58:DZ:72:ARG:HH11  | 1.74                     | 0.52              |
| 1:AA:1038:C:H2'    | 1:AA:1039:C:C6     | 2.44                     | 0.52              |
| 1:AA:192:U:H2'     | 1:AA:193:C:H6      | 1.71                     | 0.52              |
| 1:AA:658:G:O4'     | 15:AO:22:THR:HB    | 2.09                     | 0.52              |
| 2:AB:98:LEU:O      | 2:AB:101:MET:HB2   | 2.09                     | 0.52              |
| 4:AD:176:LEU:HD12  | 4:AD:177:ASP:N     | 2.24                     | 0.52              |
| 5:AE:101:ILE:N     | 5:AE:101:ILE:HD13  | 2.18                     | 0.52              |
| 5:AE:91:LEU:HD13   | 5:AE:120:THR:HG22  | 1.90                     | 0.52              |
| 7:AG:51:GLN:OE1    | 7:AG:51:GLN:HA     | 2.09                     | 0.52              |
| 10:AJ:3:LYS:HD2    | 10:AJ:77:PRO:CD    | 2.39                     | 0.52              |
| 10:AJ:79:ARG:HH11  | 10:AJ:79:ARG:N     | 2.07                     | 0.52              |
| 12:AL:78:GLN:O     | 12:AL:79:GLU:C     | 2.47                     | 0.52              |
| 24:AY:177:ILE:HG22 | 24:AY:178:ILE:N    | 2.24                     | 0.52              |
| 24:AY:517:LEU:HB3  | 24:AY:521:SER:HB2  | 1.91                     | 0.52              |
| 24:AY:689:LYS:HG3  | 24:AY:690:GLY:N    | 2.23                     | 0.52              |
| 27:B2:3:LEU:HD22   | 27:B2:7:ARG:NH2    | 2.24                     | 0.52              |
| 29:B4:48:ARG:O     | 29:B4:48:ARG:HG2   | 2.09                     | 0.52              |
| 35:BA:1683:C:H2'   | 35:BA:1684:C:C6    | 2.44                     | 0.52              |
| 35:BA:2105:C:H2'   | 35:BA:2106:G:H5'   | 1.91                     | 0.52              |
| 35:BA:2142:C:O2'   | 35:BA:2143:C:H5'   | 2.09                     | 0.52              |
| 35:BA:2461:C:O2    | 35:BA:2461:C:C2'   | 2.57                     | 0.52              |
| 35:BA:2886:G:H2'   | 35:BA:2887:U:H6    | 1.74                     | 0.52              |
| 32:B7:33:ARG:NH1   | 35:BA:467:G:OP1    | 2.42                     | 0.52              |
| 35:BA:769:G:H2'    | 35:BA:770:G:H8     | 1.75                     | 0.52              |
| 37:BC:88:GLU:CA    | 37:BC:95:VAL:HG21  | 2.40                     | 0.52              |
| 38:BD:218:ARG:HB3  | 38:BD:219:PRO:HD2  | 1.92                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 39:BE:105:THR:OG1 | 39:BE:199:ARG:NH2  | 2.43                     | 0.52              |
| 41:BG:76:SER:HA   | 41:BG:83:ARG:HB3   | 1.91                     | 0.52              |
| 41:BG:34:LEU:HD13 | 41:BG:99:MET:CE    | 2.39                     | 0.52              |
| 42:BH:118:PRO:CG  | 42:BH:121:ILE:HD12 | 2.37                     | 0.52              |
| 46:BN:35:ARG:O    | 46:BN:37:LYS:HB2   | 2.09                     | 0.52              |
| 46:BN:87:LEU:O    | 46:BN:88:GLU:C     | 2.47                     | 0.52              |
| 48:BP:9:ASN:N     | 48:BP:10:PRO:HD2   | 2.24                     | 0.52              |
| 36:BB:114:C:O2'   | 51:BS:46:VAL:HG13  | 2.09                     | 0.52              |
| 58:BZ:24:LEU:HD23 | 58:BZ:25:PRO:O     | 2.09                     | 0.52              |
| 1:CA:1369:C:H2'   | 1:CA:1370:G:H8     | 1.67                     | 0.52              |
| 1:CA:407:G:H2'    | 1:CA:408:A:H8      | 1.74                     | 0.52              |
| 1:CA:555:C:H2'    | 1:CA:556:C:C6      | 2.44                     | 0.52              |
| 5:CE:139:LEU:C    | 5:CE:141:GLN:H     | 2.13                     | 0.52              |
| 6:CF:7:ASN:OD1    | 6:CF:62:TRP:HD1    | 1.91                     | 0.52              |
| 20:CT:26:ASN:HB2  | 20:CT:71:THR:HG23  | 1.89                     | 0.52              |
| 24:CY:292:THR:HA  | 24:CY:297:GLU:O    | 2.10                     | 0.52              |
| 24:CY:359:HIS:HB2 | 24:CY:362:HIS:O    | 2.09                     | 0.52              |
| 24:CY:87:HIS:O    | 24:CY:89:ASP:N     | 2.42                     | 0.52              |
| 29:D4:16:CYS:SG   | 29:D4:17:GLY:N     | 2.83                     | 0.52              |
| 33:D8:47:LYS:HZ3  | 33:D8:49:VAL:HG13  | 1.74                     | 0.52              |
| 35:DA:1614:A:N1   | 55:DW:91:GLY:HA2   | 2.24                     | 0.52              |
| 35:DA:234:C:H2'   | 35:DA:235:U:C6     | 2.44                     | 0.52              |
| 35:DA:2478:A:H2'  | 35:DA:2479:G:O4'   | 2.09                     | 0.52              |
| 35:DA:2736:G:O2'  | 35:DA:2737:G:H5'   | 2.09                     | 0.52              |
| 35:DA:2855:C:H2'  | 35:DA:2856:C:C6    | 2.42                     | 0.52              |
| 35:DA:285:C:O2'   | 35:DA:286:C:H5''   | 2.09                     | 0.52              |
| 35:DA:302:C:P     | 57:DY:73:ARG:HH12  | 2.32                     | 0.52              |
| 38:DD:134:ARG:HG3 | 38:DD:135:PHE:HD1  | 1.74                     | 0.52              |
| 40:DF:18:ARG:C    | 40:DF:19:GLU:HG2   | 2.29                     | 0.52              |
| 42:DH:29:PRO:HD2  | 42:DH:79:VAL:O     | 2.09                     | 0.52              |
| 46:DN:78:TYR:CD1  | 46:DN:78:TYR:N     | 2.76                     | 0.52              |
| 47:DO:107:ARG:HA  | 47:DO:112:MET:CE   | 2.40                     | 0.52              |
| 48:DP:85:LEU:HD23 | 48:DP:85:LEU:N     | 2.19                     | 0.52              |
| 53:DU:61:TRP:CB   | 53:DU:93:LYS:HB3   | 2.39                     | 0.52              |
| 54:DV:25:LEU:H    | 54:DV:92:THR:HG21  | 1.74                     | 0.52              |
| 54:DV:72:VAL:HG23 | 54:DV:85:LYS:HB2   | 1.92                     | 0.52              |
| 57:DY:86:ARG:HB3  | 57:DY:88:LYS:HZ1   | 1.73                     | 0.52              |
| 57:DY:94:LYS:HG3  | 57:DY:102:CYS:SG   | 2.49                     | 0.52              |
| 1:AA:1314:C:H2'   | 1:AA:1315:U:H6     | 1.73                     | 0.52              |
| 1:AA:1375:A:H5'   | 1:AA:1376:U:OP2    | 2.10                     | 0.52              |
| 1:AA:433:C:O2'    | 1:AA:434:U:H5'     | 2.10                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:AC:134:ILE:O     | 3:AC:137:ALA:N     | 2.42                     | 0.52              |
| 3:AC:138:VAL:O     | 3:AC:139:GLN:C     | 2.48                     | 0.52              |
| 3:AC:25:GLY:O      | 3:AC:27:LYS:N      | 2.37                     | 0.52              |
| 3:AC:5:ILE:CD1     | 3:AC:5:ILE:N       | 2.72                     | 0.52              |
| 3:AC:73:PRO:O      | 3:AC:76:VAL:HG22   | 2.09                     | 0.52              |
| 4:AD:13:ARG:O      | 4:AD:16:GLY:N      | 2.36                     | 0.52              |
| 5:AE:101:ILE:HD11  | 5:AE:119:LEU:HD22  | 1.92                     | 0.52              |
| 6:AF:72:VAL:HG13   | 6:AF:73:ASN:N      | 2.24                     | 0.52              |
| 22:AV:7:G:H3'      | 22:AV:8:U:C5'      | 2.37                     | 0.52              |
| 24:AY:341:VAL:CG2  | 24:AY:350:GLU:HB2  | 2.39                     | 0.52              |
| 24:AY:411:VAL:CG1  | 24:AY:412:ALA:N    | 2.71                     | 0.52              |
| 24:AY:550:MET:HE1  | 24:AY:563:ILE:HD11 | 1.91                     | 0.52              |
| 34:B9:31:LYS:HE2   | 35:BA:2478:A:H5'   | 1.91                     | 0.52              |
| 35:BA:1015:G:H2'   | 35:BA:1016:G:H8    | 1.74                     | 0.52              |
| 35:BA:1278:A:O2'   | 35:BA:1279:G:H5'   | 2.09                     | 0.52              |
| 35:BA:135:G:O2'    | 35:BA:136:G:H5'    | 2.08                     | 0.52              |
| 35:BA:528:A:C2     | 35:BA:2043:C:C5'   | 2.92                     | 0.52              |
| 35:BA:2229:C:O2'   | 35:BA:2230:G:H5'   | 2.10                     | 0.52              |
| 35:BA:230:U:O2'    | 35:BA:231:C:H5'    | 2.09                     | 0.52              |
| 35:BA:2591:C:H2'   | 35:BA:2592:G:H8    | 1.64                     | 0.52              |
| 35:BA:2732:G:H3'   | 35:BA:2733:A:C5'   | 2.38                     | 0.52              |
| 35:BA:363(F):A:O2' | 35:BA:364:C:P      | 2.67                     | 0.52              |
| 35:BA:455:C:N3     | 35:BA:473:G:H5'    | 2.24                     | 0.52              |
| 35:BA:648:G:H2'    | 35:BA:649:G:H8     | 1.73                     | 0.52              |
| 39:BE:93:VAL:HG12  | 39:BE:175:VAL:HG21 | 1.90                     | 0.52              |
| 41:BG:27:ASN:HB3   | 41:BG:30:GLU:H     | 1.73                     | 0.52              |
| 42:BH:46:GLU:CD    | 42:BH:51:ARG:HB2   | 2.29                     | 0.52              |
| 35:BA:1063:G:O2'   | 44:BK:87:GLY:HA3   | 2.09                     | 0.52              |
| 46:BN:66:LYS:O     | 46:BN:67:LEU:HD23  | 2.08                     | 0.52              |
| 47:BO:10:VAL:HG23  | 47:BO:10:VAL:O     | 2.10                     | 0.52              |
| 48:BP:33:ARG:O     | 48:BP:35:HIS:O     | 2.26                     | 0.52              |
| 52:BT:65:LYS:HA    | 52:BT:65:LYS:HZ1   | 1.75                     | 0.52              |
| 52:BT:6:LEU:O      | 52:BT:9:LEU:N      | 2.42                     | 0.52              |
| 54:BV:37:VAL:HG23  | 54:BV:37:VAL:O     | 2.10                     | 0.52              |
| 54:BV:69:LYS:HE3   | 54:BV:71:LEU:HD21  | 1.92                     | 0.52              |
| 55:BW:59:VAL:HG21  | 55:BW:66:GLU:HB2   | 1.92                     | 0.52              |
| 57:BY:7:VAL:HB     | 57:BY:8:LYS:CE     | 2.39                     | 0.52              |
| 58:BZ:3:TYR:HD2    | 58:BZ:47:VAL:HG13  | 1.75                     | 0.52              |
| 1:CA:1314:C:H2'    | 1:CA:1315:U:H6     | 1.74                     | 0.52              |
| 1:CA:1321:C:C5'    | 1:CA:1322:C:H5'    | 2.39                     | 0.52              |
| 1:CA:1344:C:O2'    | 1:CA:1345:U:H5'    | 2.09                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:189(D):C:H2' | 1:CA:189(E):U:O4'  | 2.10                     | 0.52              |
| 1:CA:300:A:H2'    | 1:CA:301:G:O4'     | 2.08                     | 0.52              |
| 1:CA:80:G:H5''    | 1:CA:81:U:H5'      | 1.92                     | 0.52              |
| 1:CA:824:C:H2'    | 1:CA:825:G:H8      | 1.73                     | 0.52              |
| 2:CB:126:GLU:HA   | 2:CB:129:GLU:CD    | 2.29                     | 0.52              |
| 2:CB:238:LEU:HG   | 2:CB:238:LEU:O     | 2.08                     | 0.52              |
| 2:CB:33:TYR:HB2   | 2:CB:43:ASP:HB2    | 1.91                     | 0.52              |
| 12:CL:60:LEU:HD22 | 12:CL:60:LEU:N     | 2.23                     | 0.52              |
| 16:CP:9:PHE:CE2   | 16:CP:18:ARG:CZ    | 2.92                     | 0.52              |
| 22:CV:3:C:N4      | 22:CV:70:G:H1      | 2.06                     | 0.52              |
| 22:CW:65:G:H2'    | 22:CW:66:C:C1'     | 2.39                     | 0.52              |
| 24:CY:687:LEU:C   | 24:CY:688:ILE:HD12 | 2.29                     | 0.52              |
| 27:D2:48:HIS:CG   | 27:D2:49:LYS:N     | 2.76                     | 0.52              |
| 27:D2:57:ILE:O    | 27:D2:61:LEU:HG    | 2.10                     | 0.52              |
| 35:DA:1461:G:H2'  | 35:DA:1462:C:H6    | 1.74                     | 0.52              |
| 35:DA:1812:A:H2'  | 35:DA:1813:G:C8    | 2.44                     | 0.52              |
| 35:DA:2161:C:O2'  | 35:DA:2162:G:H5'   | 2.09                     | 0.52              |
| 35:DA:610:G:H22   | 35:DA:619:G:H1'    | 1.75                     | 0.52              |
| 35:DA:64:A:H2'    | 35:DA:65:C:C6      | 2.45                     | 0.52              |
| 36:DB:61:G:O2'    | 36:DB:62:C:H5'     | 2.09                     | 0.52              |
| 37:DC:60:ARG:HG2  | 37:DC:61:GLY:N     | 2.25                     | 0.52              |
| 35:DA:1829:A:N3   | 38:DD:15:PHE:HZ    | 2.08                     | 0.52              |
| 35:DA:1814:G:H4'  | 38:DD:51:VAL:HG21  | 1.91                     | 0.52              |
| 39:DE:144:ARG:O   | 39:DE:145:LYS:O    | 2.26                     | 0.52              |
| 39:DE:57:LYS:HZ3  | 39:DE:63:LEU:HG    | 1.74                     | 0.52              |
| 42:DH:92:ILE:C    | 42:DH:94:TYR:H     | 2.13                     | 0.52              |
| 48:DP:7:ARG:HA    | 48:DP:7:ARG:NH1    | 2.25                     | 0.52              |
| 51:DS:106:ARG:O   | 51:DS:107:GLU:CB   | 2.57                     | 0.52              |
| 51:DS:56:LEU:O    | 51:DS:56:LEU:HD23  | 2.08                     | 0.52              |
| 51:DS:98:VAL:C    | 51:DS:100:ALA:N    | 2.61                     | 0.52              |
| 53:DU:113:ALA:C   | 53:DU:115:ALA:N    | 2.62                     | 0.52              |
| 53:DU:84:LYS:C    | 53:DU:86:ALA:H     | 2.12                     | 0.52              |
| 53:DU:61:TRP:HB3  | 53:DU:93:LYS:HB3   | 1.90                     | 0.52              |
| 54:DV:79:VAL:O    | 54:DV:80:GLN:HB2   | 2.09                     | 0.52              |
| 35:DA:84:A:C5'    | 57:DY:9:LYS:HZ2    | 2.22                     | 0.52              |
| 1:AA:1004:A:H5'   | 1:AA:1025:U:N3     | 2.25                     | 0.52              |
| 1:AA:1058:G:H2'   | 1:AA:1059:C:C6     | 2.45                     | 0.52              |
| 1:AA:188:C:H2'    | 1:AA:189:G:C8      | 2.42                     | 0.52              |
| 1:AA:346:G:H2'    | 1:AA:347:G:O4'     | 2.10                     | 0.52              |
| 1:AA:368:U:OP1    | 24:AY:351:ARG:NH1  | 2.41                     | 0.52              |
| 1:AA:54:C:H2'     | 1:AA:352:C:N4      | 2.25                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:AB:148:TYR:O     | 2:AB:149:LEU:HD23  | 2.10                     | 0.52              |
| 2:AB:20:GLU:HB2    | 2:AB:190:THR:OG1   | 2.09                     | 0.52              |
| 7:AG:18:TYR:CD2    | 7:AG:59:LEU:HD13   | 2.44                     | 0.52              |
| 15:AO:11:VAL:O     | 15:AO:12:ILE:C     | 2.48                     | 0.52              |
| 18:AR:53:ARG:HH21  | 18:AR:59:SER:HA    | 1.74                     | 0.52              |
| 20:AT:48:LYS:HB3   | 20:AT:51:GLU:CG    | 2.38                     | 0.52              |
| 22:AV:2:G:C5'      | 25:B0:8:GLY:HA2    | 2.40                     | 0.52              |
| 24:AY:121:VAL:CG2  | 24:AY:122:TRP:H    | 2.22                     | 0.52              |
| 24:AY:438:PHE:C    | 24:AY:438:PHE:HD2  | 2.13                     | 0.52              |
| 24:AY:530:VAL:HG22 | 24:AY:531:GLY:H    | 1.73                     | 0.52              |
| 24:AY:613:PRO:C    | 24:AY:615:GLU:N    | 2.59                     | 0.52              |
| 31:B6:15:GLU:HB2   | 31:B6:47:THR:HG21  | 1.91                     | 0.52              |
| 31:B6:25:LYS:HE2   | 33:B8:34:TRP:HE1   | 1.74                     | 0.52              |
| 31:B6:9:LEU:HD12   | 31:B6:28:ARG:CG    | 2.40                     | 0.52              |
| 35:BA:1145:C:H2'   | 35:BA:1146:C:C6    | 2.45                     | 0.52              |
| 35:BA:1453:U:H2'   | 35:BA:1455:G:N7    | 2.24                     | 0.52              |
| 35:BA:246:C:H2'    | 35:BA:247:G:H5'    | 1.92                     | 0.52              |
| 35:BA:2820:A:O2'   | 35:BA:2821:A:OP1   | 2.25                     | 0.52              |
| 35:BA:285:C:O2'    | 35:BA:286:C:H5''   | 2.09                     | 0.52              |
| 35:BA:426:C:O2'    | 35:BA:427:U:H5'    | 2.09                     | 0.52              |
| 37:BC:118:PRO:HB2  | 37:BC:148:PHE:CZ   | 2.44                     | 0.52              |
| 38:BD:30:GLU:HG3   | 38:BD:63:ARG:CZ    | 2.39                     | 0.52              |
| 35:BA:1654:A:C2    | 39:BE:113:PHE:CD1  | 2.98                     | 0.52              |
| 39:BE:133:LYS:C    | 39:BE:134:ILE:HG13 | 2.29                     | 0.52              |
| 39:BE:101:ARG:NH1  | 39:BE:169:ASN:ND2  | 2.56                     | 0.52              |
| 39:BE:4:ILE:CG1    | 39:BE:5:LEU:N      | 2.72                     | 0.52              |
| 40:BF:66:PRO:O     | 40:BF:67:GLN:HB3   | 2.09                     | 0.52              |
| 46:BN:3:THR:C      | 46:BN:4:TYR:CD1    | 2.83                     | 0.52              |
| 48:BP:107:LYS:C    | 48:BP:109:GLY:N    | 2.63                     | 0.52              |
| 50:BR:10:LEU:HB3   | 50:BR:17:ARG:NE    | 2.24                     | 0.52              |
| 53:BU:56:ASP:O     | 53:BU:59:ARG:HB2   | 2.10                     | 0.52              |
| 56:BX:12:VAL:CG1   | 56:BX:27:THR:HG23  | 2.38                     | 0.52              |
| 1:CA:1261:A:C2'    | 1:CA:1262:C:H5'    | 2.39                     | 0.52              |
| 1:CA:1313:U:P      | 19:CS:6:LYS:HG3    | 2.50                     | 0.52              |
| 1:CA:1112:C:O2'    | 3:CC:179:ARG:HG2   | 2.10                     | 0.52              |
| 3:CC:15:THR:HG21   | 3:CC:181:ASN:HA    | 1.90                     | 0.52              |
| 3:CC:90:GLU:HA     | 3:CC:93:LYS:HB3    | 1.92                     | 0.52              |
| 5:CE:11:ILE:HG13   | 5:CE:33:VAL:HG23   | 1.91                     | 0.52              |
| 6:CF:15:ASP:C      | 6:CF:17:SER:N      | 2.62                     | 0.52              |
| 9:CI:104:ARG:O     | 9:CI:105:ASP:CB    | 2.56                     | 0.52              |
| 11:CK:33:THR:HB    | 11:CK:38:ASN:O     | 2.09                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 16:CP:3:LYS:HG2   | 16:CP:65:GLN:HB2   | 1.90                     | 0.52              |
| 20:CT:33:ILE:CD1  | 20:CT:63:ILE:HA    | 2.39                     | 0.52              |
| 24:CY:141:LYS:HE3 | 62:CY:703:GDP:N2   | 2.25                     | 0.52              |
| 24:CY:223:PHE:CZ  | 24:CY:249:GLY:HA3  | 2.45                     | 0.52              |
| 26:D1:86:SER:CB   | 26:D1:90:ILE:HG12  | 2.39                     | 0.52              |
| 31:D6:54:ILE:HD13 | 35:DA:2420:C:C4'   | 2.39                     | 0.52              |
| 33:D8:28:GLY:HA2  | 33:D8:32:LEU:HD21  | 1.90                     | 0.52              |
| 35:DA:2183:C:O2'  | 35:DA:2184:G:H5'   | 2.09                     | 0.52              |
| 35:DA:2348:U:C2'  | 35:DA:2349:G:C5'   | 2.87                     | 0.52              |
| 35:DA:2572:A:C8   | 39:DE:144:ARG:HB3  | 2.44                     | 0.52              |
| 35:DA:259:G:H1'   | 35:DA:621:A:O2'    | 2.08                     | 0.52              |
| 35:DA:2853:C:H2'  | 35:DA:2854:G:C8    | 2.44                     | 0.52              |
| 35:DA:493:G:H2'   | 35:DA:494:G:O4'    | 2.09                     | 0.52              |
| 35:DA:624:C:N4    | 48:DP:107:LYS:NZ   | 2.57                     | 0.52              |
| 35:DA:909:A:O2'   | 35:DA:910:A:H5'    | 2.09                     | 0.52              |
| 29:D4:3:GLU:HG3   | 36:DB:43:C:OP1     | 2.10                     | 0.52              |
| 37:DC:97:GLY:O    | 37:DC:100:ILE:HG12 | 2.09                     | 0.52              |
| 46:DN:96:GLU:CD   | 46:DN:96:GLU:N     | 2.61                     | 0.52              |
| 48:DP:9:ASN:N     | 48:DP:10:PRO:CD    | 2.73                     | 0.52              |
| 52:DT:64:ARG:HH11 | 52:DT:64:ARG:HG2   | 1.74                     | 0.52              |
| 35:DA:1248:G:N3   | 53:DU:3:ARG:HD2    | 2.25                     | 0.52              |
| 53:DU:49:HIS:C    | 53:DU:52:ARG:HB2   | 2.30                     | 0.52              |
| 53:DU:56:ASP:O    | 53:DU:59:ARG:HB2   | 2.09                     | 0.52              |
| 53:DU:57:PHE:C    | 53:DU:59:ARG:N     | 2.62                     | 0.52              |
| 2:AB:101:MET:C    | 2:AB:102:LEU:HD12  | 2.30                     | 0.52              |
| 2:AB:194:PRO:O    | 2:AB:196:LEU:N     | 2.43                     | 0.52              |
| 2:AB:187:LEU:HD23 | 2:AB:214:ILE:HG21  | 1.92                     | 0.52              |
| 3:AC:5:ILE:HD13   | 3:AC:5:ILE:N       | 2.24                     | 0.52              |
| 11:AK:111:ASP:HA  | 18:AR:84:LYS:CD    | 2.31                     | 0.52              |
| 11:AK:30:VAL:HG21 | 11:AK:65:ALA:HA    | 1.91                     | 0.52              |
| 19:AS:6:LYS:N     | 19:AS:6:LYS:HE3    | 2.25                     | 0.52              |
| 24:AY:12:LEU:HB3  | 24:AY:283:PRO:CG   | 2.39                     | 0.52              |
| 26:B1:64:ALA:C    | 26:B1:66:HIS:H     | 2.12                     | 0.52              |
| 27:B2:33:MET:O    | 27:B2:37:PHE:HD1   | 1.91                     | 0.52              |
| 29:B4:1:MET:H1    | 36:BB:43:C:H4'     | 1.75                     | 0.52              |
| 31:B6:27:LYS:HB3  | 31:B6:32:ASN:HD22  | 1.75                     | 0.52              |
| 35:BA:1080:C:H4'  | 44:BK:125:ARG:CB   | 2.40                     | 0.52              |
| 35:BA:1485:G:C1'  | 35:BA:1505:C:H42   | 2.18                     | 0.52              |
| 35:BA:1713:U:O2'  | 35:BA:1714:G:H5'   | 2.10                     | 0.52              |
| 35:BA:1754:C:OP1  | 52:BT:96:ARG:NH1   | 2.42                     | 0.52              |
| 35:BA:1821:A:H2'  | 35:BA:1822:G:H8    | 1.74                     | 0.52              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:BA:2313:C:H5'  | 35:BA:2313:C:C6    | 2.41                     | 0.52              |
| 35:BA:2347:C:H2'  | 35:BA:2348:U:C5    | 2.44                     | 0.52              |
| 35:BA:451:C:H41   | 35:BA:453:C:H3'    | 1.74                     | 0.52              |
| 35:BA:737:C:H2'   | 35:BA:738:G:H5'    | 1.91                     | 0.52              |
| 37:BC:98:GLU:O    | 37:BC:101:ILE:HD13 | 2.09                     | 0.52              |
| 39:BE:1:MET:HB2   | 39:BE:83:ASP:O     | 2.10                     | 0.52              |
| 40:BF:117:ARG:NH2 | 48:BP:5:ASP:N      | 2.58                     | 0.52              |
| 41:BG:114:ILE:O   | 41:BG:114:ILE:HG22 | 2.10                     | 0.52              |
| 43:BJ:10:UNK:O    | 43:BJ:11:UNK:CB    | 2.58                     | 0.52              |
| 44:BK:61:ALA:C    | 44:BK:63:ARG:H     | 2.13                     | 0.52              |
| 47:BO:64:ARG:HH21 | 47:BO:100:GLY:HA3  | 1.74                     | 0.52              |
| 47:BO:69:ILE:HD13 | 47:BO:77:ILE:CG2   | 2.35                     | 0.52              |
| 48:BP:85:LEU:HD23 | 48:BP:85:LEU:N     | 2.17                     | 0.52              |
| 50:BR:26:LYS:CE   | 50:BR:71:GLN:H     | 2.23                     | 0.52              |
| 50:BR:7:GLY:C     | 50:BR:8:ARG:NE     | 2.63                     | 0.52              |
| 54:BV:72:VAL:HG23 | 54:BV:85:LYS:HB2   | 1.91                     | 0.52              |
| 55:BW:1:MET:HE3   | 55:BW:2:GLU:H      | 1.75                     | 0.52              |
| 57:BY:62:GLU:CG   | 57:BY:63:LYS:N     | 2.73                     | 0.52              |
| 57:BY:77:PRO:O    | 57:BY:99:CYS:SG    | 2.61                     | 0.52              |
| 57:BY:97:ARG:HG3  | 57:BY:97:ARG:NH1   | 2.24                     | 0.52              |
| 1:CA:1002:G:N2    | 1:CA:1039:C:H2'    | 2.25                     | 0.52              |
| 1:CA:1347:G:O2'   | 1:CA:1348:U:OP2    | 2.28                     | 0.52              |
| 1:CA:423:G:C2'    | 1:CA:424:G:H5'     | 2.40                     | 0.52              |
| 1:CA:956:U:H2'    | 1:CA:957:U:H6      | 1.74                     | 0.52              |
| 1:CA:998:G:H2'    | 1:CA:999:C:N1      | 2.24                     | 0.52              |
| 3:CC:5:ILE:CD1    | 3:CC:5:ILE:N       | 2.72                     | 0.52              |
| 6:CF:62:TRP:O     | 6:CF:63:TYR:CG     | 2.63                     | 0.52              |
| 1:CA:1378:C:O2    | 7:CG:76:ARG:NH2    | 2.43                     | 0.52              |
| 12:CL:46:LYS:HB2  | 12:CL:92:ASP:O     | 2.09                     | 0.52              |
| 19:CS:13:ASP:C    | 19:CS:15:LEU:N     | 2.63                     | 0.52              |
| 33:D8:53:PRO:HA   | 33:D8:56:GLU:HB2   | 1.92                     | 0.52              |
| 35:DA:1204:A:H61  | 35:DA:1240:U:H2'   | 1.73                     | 0.52              |
| 35:DA:1782:C:H2'  | 35:DA:1783:A:H5'   | 1.92                     | 0.52              |
| 35:DA:1839:G:N3   | 35:DA:1839:G:H2'   | 2.24                     | 0.52              |
| 35:DA:194:G:H2'   | 35:DA:195:A:O4'    | 2.10                     | 0.52              |
| 35:DA:1985:G:O2'  | 35:DA:1986:A:H5'   | 2.09                     | 0.52              |
| 30:D5:10:LYS:HB2  | 35:DA:2017:U:O2    | 2.10                     | 0.52              |
| 35:DA:2121:G:O2'  | 37:DC:168:LYS:HG2  | 2.09                     | 0.52              |
| 35:DA:272(I):U:H5 | 35:DA:363(A):A:H2  | 1.57                     | 0.52              |
| 35:DA:2771:C:H2'  | 35:DA:2772:C:C6    | 2.45                     | 0.52              |
| 35:DA:548:A:C3'   | 35:DA:549:G:H5'    | 2.39                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:DD:209:ALA:C    | 38:DD:210:GLY:O    | 2.46                     | 0.52              |
| 39:DE:51:PHE:CD1   | 39:DE:52:LEU:N     | 2.78                     | 0.52              |
| 35:DA:1205:U:C5    | 40:DF:171:PRO:HA   | 2.45                     | 0.52              |
| 35:DA:675:A:H4'    | 40:DF:67:GLN:OE1   | 2.08                     | 0.52              |
| 44:DK:61:ALA:C     | 44:DK:63:ARG:H     | 2.12                     | 0.52              |
| 46:DN:49:GLY:CA    | 46:DN:119:ARG:HH12 | 2.22                     | 0.52              |
| 47:DO:104:ARG:NH2  | 52:DT:33:LYS:HE3   | 2.24                     | 0.52              |
| 48:DP:85:LEU:HD12  | 48:DP:120:ALA:CB   | 2.33                     | 0.52              |
| 49:DQ:67:ARG:HD2   | 49:DQ:105:GLU:OE1  | 2.10                     | 0.52              |
| 49:DQ:12:GLN:NE2   | 49:DQ:72:LYS:HG3   | 2.25                     | 0.52              |
| 54:DV:93:GLU:O     | 54:DV:94:LEU:HD23  | 2.10                     | 0.52              |
| 56:DX:63:LYS:HA    | 56:DX:72:LYS:HA    | 1.90                     | 0.52              |
| 1:AA:1026:G:C3'    | 1:AA:1027:C:H5'    | 2.40                     | 0.52              |
| 1:AA:1351:U:O4'    | 7:AG:33:ASP:HB3    | 2.09                     | 0.52              |
| 1:AA:189(A):C:H2'  | 1:AA:189(B):C:H6   | 1.74                     | 0.52              |
| 1:AA:418:C:H2'     | 1:AA:419:C:C6      | 2.45                     | 0.52              |
| 1:AA:423:G:H2'     | 1:AA:424:G:H5'     | 1.91                     | 0.52              |
| 4:AD:107:ARG:HH21  | 4:AD:194:LEU:HD12  | 1.75                     | 0.52              |
| 4:AD:196:LEU:C     | 4:AD:198:VAL:H     | 2.12                     | 0.52              |
| 9:AI:69:GLY:O      | 9:AI:73:GLN:HG3    | 2.10                     | 0.52              |
| 13:AM:119:GLY:O    | 13:AM:120:LYS:HB2  | 2.10                     | 0.52              |
| 16:AP:19:ILE:N     | 16:AP:37:GLY:O     | 2.39                     | 0.52              |
| 19:AS:31:ILE:O     | 19:AS:31:ILE:HG23  | 2.10                     | 0.52              |
| 19:AS:41:VAL:O     | 19:AS:41:VAL:HG23  | 2.09                     | 0.52              |
| 24:AY:282:SER:O    | 24:AY:284:LEU:N    | 2.43                     | 0.52              |
| 24:AY:486:THR:HG23 | 24:AY:600:VAL:HG13 | 1.91                     | 0.52              |
| 26:B1:68:PRO:C     | 26:B1:70:VAL:H     | 2.13                     | 0.52              |
| 27:B2:7:ARG:HG3    | 27:B2:7:ARG:HH11   | 1.73                     | 0.52              |
| 28:B3:15:TYR:HD2   | 28:B3:19:GLN:HE22  | 1.57                     | 0.52              |
| 28:B3:56:VAL:CG1   | 28:B3:57:GLU:N     | 2.73                     | 0.52              |
| 31:B6:27:LYS:CD    | 31:B6:27:LYS:O     | 2.55                     | 0.52              |
| 32:B7:46:VAL:CG1   | 32:B7:47:ARG:N     | 2.73                     | 0.52              |
| 35:BA:1491:G:N2    | 35:BA:1492:G:H1'   | 2.24                     | 0.52              |
| 35:BA:1542:A:H8    | 35:BA:1542:A:H3'   | 1.74                     | 0.52              |
| 35:BA:154(A):C:H3' | 35:BA:155:U:H5''   | 1.92                     | 0.52              |
| 35:BA:1624:G:O2'   | 35:BA:1625:C:H5'   | 2.10                     | 0.52              |
| 35:BA:1819:A:H1'   | 35:BA:1821:A:C6    | 2.45                     | 0.52              |
| 35:BA:1865:G:C2'   | 35:BA:1866:C:H5''  | 2.40                     | 0.52              |
| 31:B6:37:ARG:NH2   | 35:BA:2286:A:N6    | 2.58                     | 0.52              |
| 35:BA:2816:C:O2    | 35:BA:2883:A:O2'   | 2.28                     | 0.52              |
| 35:BA:402:A:O2'    | 35:BA:403:U:H5'    | 2.10                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:BH:159:GLU:O    | 42:BH:160:LYS:O    | 2.26                     | 0.52              |
| 48:BP:99:LEU:HA    | 48:BP:102:ARG:HH12 | 1.74                     | 0.52              |
| 48:BP:83:VAL:HG11  | 48:BP:112:LEU:HD21 | 1.91                     | 0.52              |
| 48:BP:62:LEU:HD22  | 48:BP:62:LEU:H     | 1.71                     | 0.52              |
| 48:BP:98:GLU:O     | 48:BP:101:VAL:HG22 | 2.10                     | 0.52              |
| 52:BT:56:GLY:O     | 52:BT:59:THR:HG23  | 2.10                     | 0.52              |
| 1:CA:452:A:O2'     | 1:CA:453:A:H8      | 1.91                     | 0.52              |
| 1:CA:630:G:H2'     | 1:CA:631:G:H5''    | 1.85                     | 0.52              |
| 1:CA:680:C:O2'     | 1:CA:681:C:H5'     | 2.10                     | 0.52              |
| 1:CA:818:G:O2'     | 1:CA:819:A:H5'     | 2.10                     | 0.52              |
| 1:CA:972:C:H4'     | 10:CJ:57:LYS:CB    | 2.40                     | 0.52              |
| 2:CB:115:LEU:HD13  | 2:CB:145:LEU:HB3   | 1.91                     | 0.52              |
| 2:CB:121:LEU:HA    | 2:CB:124:SER:HB3   | 1.92                     | 0.52              |
| 4:CD:9:CYS:HB3     | 4:CD:32:ALA:HB2    | 1.90                     | 0.52              |
| 5:CE:142:LEU:O     | 5:CE:143:ARG:NE    | 2.43                     | 0.52              |
| 9:CI:95:LYS:HD3    | 9:CI:95:LYS:C      | 2.29                     | 0.52              |
| 10:CJ:55:LYS:CE    | 10:CJ:55:LYS:N     | 2.63                     | 0.52              |
| 16:CP:50:LYS:HG2   | 16:CP:51:VAL:H     | 1.74                     | 0.52              |
| 19:CS:19:VAL:CG1   | 19:CS:44:MET:HG2   | 2.40                     | 0.52              |
| 22:CW:52:C:H2'     | 22:CW:53:G:H5''    | 1.91                     | 0.52              |
| 24:CY:334:THR:CG2  | 24:CY:368:GLU:HB2  | 2.40                     | 0.52              |
| 61:CY:702:FUA:H201 | 61:CY:702:FUA:O1   | 2.09                     | 0.52              |
| 29:D4:53:GLU:OE1   | 29:D4:55:ARG:HD3   | 2.09                     | 0.52              |
| 30:D5:45:VAL:HG22  | 30:D5:51:TYR:CD1   | 2.44                     | 0.52              |
| 31:D6:41:PRO:O     | 31:D6:42:TRP:C     | 2.48                     | 0.52              |
| 34:D9:4:ARG:HH12   | 35:DA:2477:C:N4    | 2.07                     | 0.52              |
| 35:DA:123:G:O2'    | 35:DA:124:G:H5'    | 2.10                     | 0.52              |
| 35:DA:134:C:H2'    | 35:DA:135:G:C8     | 2.44                     | 0.52              |
| 35:DA:1865:G:C2'   | 35:DA:1866:C:H5''  | 2.40                     | 0.52              |
| 35:DA:1908:C:H2'   | 35:DA:1909:C:H6    | 1.74                     | 0.52              |
| 35:DA:1983:C:O2'   | 35:DA:1984:G:H5'   | 2.10                     | 0.52              |
| 35:DA:2105:C:H2'   | 35:DA:2106:G:H5'   | 1.91                     | 0.52              |
| 35:DA:455:C:N3     | 35:DA:473:G:H5'    | 2.25                     | 0.52              |
| 38:DD:39:LYS:HZ2   | 38:DD:87:ASN:HB3   | 1.74                     | 0.52              |
| 41:DG:101:ILE:O    | 41:DG:104:GLU:HB3  | 2.10                     | 0.52              |
| 41:DG:131:TYR:CE2  | 41:DG:133:LEU:HD23 | 2.39                     | 0.52              |
| 46:DN:15:LEU:HD12  | 46:DN:136:GLU:HG3  | 1.92                     | 0.52              |
| 47:DO:61:VAL:HG21  | 47:DO:111:PHE:CE2  | 2.45                     | 0.52              |
| 48:DP:13:ASN:O     | 48:DP:14:LYS:CB    | 2.57                     | 0.52              |
| 35:DA:2415:G:H4'   | 48:DP:66:GLY:C     | 2.29                     | 0.52              |
| 50:DR:10:LEU:HB3   | 50:DR:17:ARG:NE    | 2.25                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:DS:26:LEU:O     | 51:DS:88:ASP:HB3   | 2.10                     | 0.52              |
| 55:DW:88:ARG:HD3   | 55:DW:94:ASP:OD1   | 2.09                     | 0.52              |
| 58:DZ:81:ARG:HH11  | 58:DZ:81:ARG:HB3   | 1.73                     | 0.52              |
| 1:AA:1129:C:H5'    | 1:AA:1129:C:C6     | 2.44                     | 0.52              |
| 1:AA:1347:G:HO2'   | 1:AA:1373:G:H1     | 1.58                     | 0.52              |
| 1:AA:1409:C:O2'    | 1:AA:1410:G:H5'    | 2.10                     | 0.52              |
| 1:AA:490:G:H2'     | 1:AA:491:G:C8      | 2.41                     | 0.52              |
| 3:AC:15:THR:CG2    | 3:AC:181:ASN:HA    | 2.40                     | 0.52              |
| 4:AD:120:LEU:HB3   | 4:AD:126:ILE:HD11  | 1.92                     | 0.52              |
| 7:AG:69:VAL:HG21   | 7:AG:104:LEU:HD21  | 1.92                     | 0.52              |
| 8:AH:41:ARG:NH2    | 8:AH:123:GLU:CD    | 2.63                     | 0.52              |
| 9:AI:93:ARG:HA     | 9:AI:96:LEU:HB2    | 1.91                     | 0.52              |
| 10:AJ:82:ILE:O     | 10:AJ:86:MET:CB    | 2.58                     | 0.52              |
| 15:AO:65:ARG:NH1   | 15:AO:65:ARG:HG2   | 2.25                     | 0.52              |
| 18:AR:37:VAL:HG23  | 18:AR:38:GLU:HG2   | 1.91                     | 0.52              |
| 1:AA:187:C:OP1     | 20:AT:82:SER:HB2   | 2.08                     | 0.52              |
| 22:AW:12:G:N2      | 22:AW:13:C:H1'     | 2.25                     | 0.52              |
| 22:AW:1:C:H2'      | 22:AW:2:G:C8       | 2.40                     | 0.52              |
| 24:AY:180:VAL:HG23 | 24:AY:216:LEU:CD1  | 2.37                     | 0.52              |
| 24:AY:35:TYR:HH    | 24:AY:266:ASN:HB3  | 1.72                     | 0.52              |
| 24:AY:340:TYR:CE1  | 24:AY:351:ARG:HB2  | 2.45                     | 0.52              |
| 24:AY:413:ILE:HD11 | 24:AY:474:ALA:HB3  | 1.92                     | 0.52              |
| 28:B3:17:LYS:HZ2   | 28:B3:20:LYS:HE3   | 1.74                     | 0.52              |
| 34:B9:29:ASN:H     | 34:B9:29:ASN:ND2   | 2.07                     | 0.52              |
| 35:BA:1400:G:H2'   | 35:BA:1401:G:C8    | 2.44                     | 0.52              |
| 35:BA:1853:A:H2'   | 35:BA:1854:A:C8    | 2.44                     | 0.52              |
| 35:BA:881:G:C2'    | 35:BA:882:G:H5'    | 2.39                     | 0.52              |
| 35:BA:7:G:O2'      | 35:BA:8:A:H5'      | 2.10                     | 0.52              |
| 39:BE:116:VAL:HG21 | 39:BE:122:PHE:CD2  | 2.45                     | 0.52              |
| 40:BF:110:LEU:CD1  | 40:BF:206:ILE:HD11 | 2.31                     | 0.52              |
| 40:BF:9:ILE:HG12   | 40:BF:15:SER:N     | 2.24                     | 0.52              |
| 46:BN:74:ARG:NH2   | 46:BN:83:LYS:HD3   | 2.24                     | 0.52              |
| 47:BO:63:VAL:O     | 47:BO:64:ARG:HG2   | 2.10                     | 0.52              |
| 48:BP:102:ARG:O    | 48:BP:102:ARG:HG2  | 2.09                     | 0.52              |
| 33:B8:13:ARG:HB3   | 48:BP:63:PRO:HB3   | 1.91                     | 0.52              |
| 49:BQ:12:GLN:NE2   | 49:BQ:72:LYS:HG3   | 2.24                     | 0.52              |
| 35:BA:1654:A:P     | 50:BR:3:HIS:HB2    | 2.49                     | 0.52              |
| 50:BR:4:LEU:C      | 50:BR:6:SER:H      | 2.13                     | 0.52              |
| 51:BS:51:ALA:HB3   | 51:BS:73:LEU:HB2   | 1.92                     | 0.52              |
| 55:BW:88:ARG:HD3   | 55:BW:94:ASP:OD1   | 2.09                     | 0.52              |
| 1:CA:155:C:H2'     | 1:CA:156:G:H8      | 1.75                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:560:U:H4'     | 1:CA:561:U:H5''    | 1.92                     | 0.52              |
| 1:CA:738:C:H5''    | 6:CF:69:GLU:HB2    | 1.91                     | 0.52              |
| 4:CD:17:VAL:O      | 4:CD:18:LYS:O      | 2.27                     | 0.52              |
| 10:CJ:33:GLN:HB2   | 10:CJ:75:ILE:HD13  | 1.91                     | 0.52              |
| 15:CO:74:ASP:OD2   | 15:CO:77:ARG:HG2   | 2.09                     | 0.52              |
| 24:CY:33:LEU:CD2   | 24:CY:360:ALA:HB2  | 2.27                     | 0.52              |
| 24:CY:374:LEU:HD12 | 24:CY:374:LEU:N    | 2.25                     | 0.52              |
| 24:CY:441:SER:O    | 24:CY:449:THR:HA   | 2.09                     | 0.52              |
| 24:CY:509:HIS:O    | 24:CY:510:VAL:HG23 | 2.10                     | 0.52              |
| 25:D0:23:VAL:HG11  | 25:D0:69:PHE:HZ    | 1.75                     | 0.52              |
| 31:D6:24:GLU:OE2   | 35:DA:2346:A:H8    | 1.93                     | 0.52              |
| 31:D6:9:LEU:HD22   | 31:D6:9:LEU:O      | 2.10                     | 0.52              |
| 32:D7:17:GLY:O     | 32:D7:20:ALA:HB3   | 2.10                     | 0.52              |
| 35:DA:1516:C:C2'   | 35:DA:1517:G:C5'   | 2.87                     | 0.52              |
| 35:DA:142(A):C:O2' | 35:DA:1597:A:H5''  | 2.09                     | 0.52              |
| 35:DA:1666:G:C2'   | 35:DA:1667:G:H5'   | 2.39                     | 0.52              |
| 35:DA:2019:A:O4'   | 53:DU:34:LYS:HD2   | 2.09                     | 0.52              |
| 35:DA:2220:G:H2'   | 35:DA:2221:G:H8    | 1.75                     | 0.52              |
| 35:DA:2307:G:N2    | 35:DA:2308:G:C5'   | 2.72                     | 0.52              |
| 35:DA:271(E):U:H2' | 35:DA:271(F):C:C6  | 2.44                     | 0.52              |
| 35:DA:2870:C:O2'   | 35:DA:2871:C:H5'   | 2.08                     | 0.52              |
| 35:DA:841:A:H5'    | 35:DA:841:A:H8     | 1.73                     | 0.52              |
| 38:DD:248:SER:HB2  | 38:DD:249:PRO:HD2  | 1.92                     | 0.52              |
| 35:DA:1568:G:P     | 38:DD:63:ARG:HH22  | 2.32                     | 0.52              |
| 39:DE:117:MET:HA   | 39:DE:122:PHE:N    | 2.13                     | 0.52              |
| 40:DF:117:ARG:NH2  | 48:DP:5:ASP:N      | 2.58                     | 0.52              |
| 40:DF:50:SER:HB2   | 40:DF:94:PRO:HD3   | 1.92                     | 0.52              |
| 41:DG:139:LEU:HA   | 41:DG:144:ILE:HD13 | 1.92                     | 0.52              |
| 41:DG:133:LEU:CD1  | 41:DG:157:ILE:HD12 | 2.39                     | 0.52              |
| 41:DG:40:ASN:ND2   | 41:DG:90:LEU:O     | 2.42                     | 0.52              |
| 41:DG:55:LYS:C     | 41:DG:57:ALA:N     | 2.63                     | 0.52              |
| 41:DG:82:LEU:HD13  | 41:DG:87:PRO:CB    | 2.39                     | 0.52              |
| 44:DK:74:ALA:HB2   | 44:DK:111:LYS:HE2  | 1.92                     | 0.52              |
| 46:DN:10:GLU:CD    | 46:DN:11:PRO:HD2   | 2.30                     | 0.52              |
| 46:DN:137:LYS:O    | 46:DN:138:LEU:HD23 | 2.09                     | 0.52              |
| 46:DN:58:ASP:O     | 46:DN:60:ILE:HG13  | 2.09                     | 0.52              |
| 48:DP:39:LYS:HE2   | 48:DP:40:SER:N     | 2.17                     | 0.52              |
| 50:DR:117:VAL:O    | 50:DR:118:GLU:CB   | 2.56                     | 0.52              |
| 50:DR:28:LEU:HD22  | 50:DR:29:LEU:HD12  | 1.92                     | 0.52              |
| 50:DR:4:LEU:C      | 50:DR:6:SER:N      | 2.63                     | 0.52              |
| 54:DV:2:PHE:CE1    | 54:DV:13:ARG:NH1   | 2.77                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 55:DW:14:PRO:HG2  | 55:DW:78:GLU:HB2   | 1.91                     | 0.52              |
| 55:DW:20:VAL:HG23 | 55:DW:47:VAL:HG21  | 1.91                     | 0.52              |
| 35:DA:65:C:H5'    | 56:DX:71:GLY:HA3   | 1.91                     | 0.52              |
| 1:AA:1303:C:N4    | 1:AA:1304:G:C6     | 2.78                     | 0.52              |
| 1:AA:1368:G:C2'   | 1:AA:1369:C:H5'    | 2.40                     | 0.52              |
| 1:AA:352:C:H4'    | 1:AA:354:G:OP1     | 2.10                     | 0.52              |
| 1:AA:383:A:C2'    | 1:AA:384:G:H5'     | 2.40                     | 0.52              |
| 6:AF:45:LEU:O     | 6:AF:46:ARG:CG     | 2.56                     | 0.52              |
| 6:AF:44:GLY:HA2   | 6:AF:59:TYR:CE1    | 2.45                     | 0.52              |
| 7:AG:120:ILE:HG22 | 7:AG:124:LEU:CD1   | 2.39                     | 0.52              |
| 9:AI:48:GLU:N     | 9:AI:49:PRO:CD     | 2.73                     | 0.52              |
| 9:AI:79:LEU:HD11  | 9:AI:83:ARG:CD     | 2.40                     | 0.52              |
| 10:AJ:55:LYS:HE3  | 10:AJ:55:LYS:N     | 2.25                     | 0.52              |
| 10:AJ:3:LYS:HG3   | 10:AJ:75:ILE:O     | 2.10                     | 0.52              |
| 12:AL:86:ARG:O    | 12:AL:86:ARG:HG2   | 2.08                     | 0.52              |
| 13:AM:54:VAL:HG12 | 13:AM:58:GLU:HG2   | 1.91                     | 0.52              |
| 16:AP:4:ILE:HG13  | 16:AP:64:ALA:HB1   | 1.92                     | 0.52              |
| 20:AT:26:ASN:HB2  | 20:AT:71:THR:HG23  | 1.92                     | 0.52              |
| 24:AY:19:ALA:HA   | 24:AY:121:VAL:HG11 | 1.91                     | 0.52              |
| 26:B1:86:SER:O    | 26:B1:90:ILE:N     | 2.43                     | 0.52              |
| 27:B2:38:GLN:HA   | 27:B2:41:ILE:HG23  | 1.91                     | 0.52              |
| 30:B5:41:PRO:O    | 30:B5:44:THR:OG1   | 2.20                     | 0.52              |
| 30:B5:45:VAL:HG22 | 30:B5:51:TYR:CD1   | 2.44                     | 0.52              |
| 35:BA:1040:C:C4   | 35:BA:1041:C:C4    | 2.98                     | 0.52              |
| 35:BA:1097:U:H2'  | 35:BA:1098:A:H5'   | 1.91                     | 0.52              |
| 35:BA:1204:A:N1   | 35:BA:1241:A:H2    | 2.07                     | 0.52              |
| 35:BA:1913:A:H4'  | 35:BA:1914:C:H5''  | 1.92                     | 0.52              |
| 35:BA:2776:A:H4'  | 35:BA:2777:G:H5''  | 1.92                     | 0.52              |
| 35:BA:259:G:H1'   | 35:BA:621:A:O2'    | 2.09                     | 0.52              |
| 37:BC:42:VAL:O    | 37:BC:176:VAL:HG22 | 2.10                     | 0.52              |
| 39:BE:10:GLY:HA2  | 39:BE:192:ASN:HD21 | 1.75                     | 0.52              |
| 41:BG:62:LEU:HD12 | 41:BG:62:LEU:N     | 2.23                     | 0.52              |
| 48:BP:107:LYS:HG3 | 48:BP:107:LYS:O    | 2.10                     | 0.52              |
| 35:BA:941:A:H4'   | 48:BP:35:HIS:HE1   | 1.74                     | 0.52              |
| 48:BP:89:ALA:HA   | 48:BP:121:LYS:HD3  | 1.91                     | 0.52              |
| 49:BQ:97:VAL:HG11 | 49:BQ:103:MET:HE1  | 1.90                     | 0.52              |
| 52:BT:50:ILE:CG1  | 52:BT:102:ILE:HD11 | 2.40                     | 0.52              |
| 54:BV:99:ILE:N    | 54:BV:99:ILE:HD13  | 2.25                     | 0.52              |
| 56:BX:10:ALA:HB1  | 56:BX:11:PRO:CD    | 2.40                     | 0.52              |
| 56:BX:55:ASN:HB2  | 56:BX:80:ILE:HG12  | 1.91                     | 0.52              |
| 56:BX:63:LYS:HA   | 56:BX:72:LYS:HA    | 1.91                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:164:U:H2'    | 1:CA:165:C:C6      | 2.44                     | 0.52              |
| 1:CA:297:G:H4'    | 1:CA:557:G:H4'     | 1.92                     | 0.52              |
| 1:CA:352:C:H4'    | 1:CA:354:G:OP1     | 2.08                     | 0.52              |
| 1:CA:715:A:H2'    | 1:CA:716:A:H8      | 1.75                     | 0.52              |
| 1:CA:781:A:H2'    | 1:CA:782:A:H5'     | 1.90                     | 0.52              |
| 2:CB:189:ASP:O    | 2:CB:191:ASP:N     | 2.43                     | 0.52              |
| 3:CC:72:LYS:HE3   | 3:CC:72:LYS:HA     | 1.92                     | 0.52              |
| 5:CE:76:ILE:CG2   | 5:CE:118:ILE:HD13  | 2.40                     | 0.52              |
| 17:CQ:66:SER:O    | 17:CQ:70:ARG:NH1   | 2.43                     | 0.52              |
| 1:CA:263:A:OP2    | 20:CT:79:ARG:NH1   | 2.43                     | 0.52              |
| 22:CV:9:G:O2'     | 22:CV:10:G:N7      | 2.35                     | 0.52              |
| 22:CW:16:C:O2     | 22:CW:61:U:H4'     | 2.10                     | 0.52              |
| 24:CY:152:THR:CG2 | 24:CY:153:MET:N    | 2.73                     | 0.52              |
| 24:CY:15:ILE:HD12 | 24:CY:81:ILE:HG23  | 1.90                     | 0.52              |
| 24:CY:236:GLU:HG3 | 24:CY:236:GLU:O    | 2.08                     | 0.52              |
| 24:CY:68:ALA:HB3  | 24:CY:327:PHE:CD1  | 2.45                     | 0.52              |
| 25:D0:74:ARG:HG2  | 36:DB:13:A:OP2     | 2.10                     | 0.52              |
| 31:D6:10:LEU:HB3  | 33:D8:34:TRP:HD1   | 1.75                     | 0.52              |
| 31:D6:13:CYS:HB3  | 31:D6:49:HIS:HB3   | 1.91                     | 0.52              |
| 33:D8:51:ALA:HA   | 33:D8:54:GLU:OE1   | 2.09                     | 0.52              |
| 35:DA:1432:C:H2'  | 35:DA:1433:U:O4'   | 2.09                     | 0.52              |
| 35:DA:1453:U:H2'  | 35:DA:1455:G:N7    | 2.25                     | 0.52              |
| 35:DA:2118:U:OP1  | 35:DA:2148:G:H4'   | 2.10                     | 0.52              |
| 35:DA:2691:C:H6   | 35:DA:2691:C:H5'   | 1.75                     | 0.52              |
| 35:DA:514:A:H2'   | 35:DA:515:A:H8     | 1.73                     | 0.52              |
| 37:DC:120:VAL:O   | 37:DC:124:VAL:HG23 | 2.10                     | 0.52              |
| 35:DA:2177:C:O2   | 37:DC:173:HIS:HE1  | 1.92                     | 0.52              |
| 35:DA:1654:A:H2   | 39:DE:113:PHE:CD1  | 2.28                     | 0.52              |
| 39:DE:176:ILE:CG2 | 39:DE:178:GLU:HB3  | 2.36                     | 0.52              |
| 39:DE:10:GLY:HA2  | 39:DE:192:ASN:HD21 | 1.75                     | 0.52              |
| 39:DE:38:THR:CB   | 39:DE:41:LYS:HG2   | 2.32                     | 0.52              |
| 39:DE:77:ILE:C    | 39:DE:78:LEU:HG    | 2.30                     | 0.52              |
| 46:DN:35:ARG:O    | 46:DN:37:LYS:HB2   | 2.09                     | 0.52              |
| 46:DN:3:THR:C     | 46:DN:4:TYR:CD1    | 2.83                     | 0.52              |
| 50:DR:53:HIS:O    | 50:DR:53:HIS:ND1   | 2.42                     | 0.52              |
| 51:DS:30:ARG:HH22 | 51:DS:62:LYS:HD2   | 1.75                     | 0.52              |
| 53:DU:99:ALA:HB2  | 53:DU:106:PHE:CE1  | 2.44                     | 0.52              |
| 53:DU:26:GLY:C    | 53:DU:28:ARG:H     | 2.14                     | 0.52              |
| 54:DV:16:PRO:O    | 54:DV:96:ILE:O     | 2.28                     | 0.52              |
| 57:DY:7:VAL:HB    | 57:DY:8:LYS:CE     | 2.40                     | 0.52              |
| 57:DY:96:ILE:CD1  | 57:DY:99:CYS:SG    | 2.98                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:375:U:H4'     | 16:AP:17:TYR:CE2   | 2.45                     | 0.52              |
| 1:AA:658:G:H2'     | 1:AA:659:U:C6      | 2.45                     | 0.52              |
| 4:AD:36:ARG:HH11   | 4:AD:36:ARG:CG     | 2.23                     | 0.52              |
| 8:AH:64:LYS:HD2    | 8:AH:79:VAL:HG21   | 1.92                     | 0.52              |
| 10:AJ:32:ALA:N     | 10:AJ:78:ASN:HD21  | 2.06                     | 0.52              |
| 15:AO:53:HIS:O     | 15:AO:56:LEU:HB3   | 2.10                     | 0.52              |
| 1:AA:1313:U:OP2    | 19:AS:6:LYS:CB     | 2.58                     | 0.52              |
| 24:AY:12:LEU:CB    | 24:AY:283:PRO:HG2  | 2.39                     | 0.52              |
| 24:AY:373:ASP:C    | 24:AY:374:LEU:HD12 | 2.29                     | 0.52              |
| 24:AY:86:GLY:O     | 24:AY:88:VAL:HG22  | 2.09                     | 0.52              |
| 25:B0:20:ARG:HG2   | 25:B0:20:ARG:HH11  | 1.75                     | 0.52              |
| 27:B2:53:LEU:O     | 27:B2:53:LEU:HD23  | 2.09                     | 0.52              |
| 28:B3:28:LEU:CD2   | 28:B3:35:ARG:HD2   | 2.40                     | 0.52              |
| 29:B4:31:ILE:CG2   | 29:B4:33:VAL:HG23  | 2.39                     | 0.52              |
| 30:B5:39:MET:HG3   | 55:BW:34:ASN:ND2   | 2.25                     | 0.52              |
| 31:B6:27:LYS:HZ2   | 31:B6:30:THR:HB    | 1.75                     | 0.52              |
| 35:BA:1930:G:N2    | 35:BA:1968:G:H2'   | 2.25                     | 0.52              |
| 35:BA:677:A:H4'    | 35:BA:2070:G:O2'   | 2.10                     | 0.52              |
| 35:BA:2373:G:H2'   | 35:BA:2374:C:C6    | 2.45                     | 0.52              |
| 26:B1:30:VAL:H     | 35:BA:2396:G:H4'   | 1.73                     | 0.52              |
| 35:BA:2461:C:H42   | 35:BA:2489:G:H1    | 1.58                     | 0.52              |
| 35:BA:2590:A:OP2   | 38:BD:238:GLY:HA2  | 2.10                     | 0.52              |
| 35:BA:2747:G:H21   | 35:BA:2757:A:H62   | 1.56                     | 0.52              |
| 35:BA:634:C:H2'    | 35:BA:635:C:C6     | 2.45                     | 0.52              |
| 36:BB:29:A:H3'     | 51:BS:32:LEU:HD11  | 1.92                     | 0.52              |
| 40:BF:100:THR:O    | 40:BF:100:THR:HG22 | 2.08                     | 0.52              |
| 40:BF:9:ILE:HG12   | 40:BF:14:PRO:C     | 2.30                     | 0.52              |
| 43:BJ:6:UNK:O      | 43:BJ:8:UNK:N      | 2.43                     | 0.52              |
| 44:BK:132:ARG:HG3  | 44:BK:132:ARG:HH11 | 1.74                     | 0.52              |
| 48:BP:101:VAL:HG12 | 48:BP:106:LEU:CB   | 2.40                     | 0.52              |
| 50:BR:12:ARG:HB3   | 50:BR:16:HIS:CD2   | 2.45                     | 0.52              |
| 50:BR:28:LEU:HD22  | 50:BR:29:LEU:HD12  | 1.91                     | 0.52              |
| 52:BT:55:ASN:HD22  | 52:BT:58:ASN:ND2   | 2.07                     | 0.52              |
| 54:BV:49:THR:HB    | 54:BV:50:PRO:HD2   | 1.92                     | 0.52              |
| 1:CA:1495:U:C2     | 1:CA:1496:C:C5     | 2.97                     | 0.52              |
| 1:CA:509:A:N1      | 1:CA:510:A:C2      | 2.78                     | 0.52              |
| 4:CD:2:GLY:O       | 4:CD:4:TYR:N       | 2.43                     | 0.52              |
| 7:CG:78:ARG:HH11   | 7:CG:78:ARG:HG3    | 1.75                     | 0.52              |
| 8:CH:6:ILE:H       | 8:CH:6:ILE:CD1     | 2.23                     | 0.52              |
| 10:CJ:92:THR:HG23  | 10:CJ:93:GLY:N     | 2.24                     | 0.52              |
| 12:CL:23:LYS:HE3   | 12:CL:89:ARG:HE    | 1.75                     | 0.52              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:CM:80:ARG:O     | 13:CM:83:ASP:HB3   | 2.10                     | 0.52              |
| 13:CM:9:ILE:N      | 13:CM:9:ILE:HD12   | 2.25                     | 0.52              |
| 20:CT:33:ILE:HD13  | 20:CT:63:ILE:HA    | 1.90                     | 0.52              |
| 22:CV:36:U:O2      | 24:CY:502:GLY:HA2  | 2.10                     | 0.52              |
| 22:CW:14:A:C2'     | 22:CW:15:G:H5''    | 2.40                     | 0.52              |
| 22:CW:20:G:H4'     | 22:CW:21:U:OP2     | 2.09                     | 0.52              |
| 30:D5:42:PRO:HB2   | 30:D5:43:HIS:CD2   | 2.45                     | 0.52              |
| 30:D5:48:GLU:O     | 30:D5:49:CYS:SG    | 2.68                     | 0.52              |
| 35:DA:1231:G:H2'   | 35:DA:1232:G:C8    | 2.45                     | 0.52              |
| 35:DA:154(A):C:N4  | 35:DA:172:C:H42    | 2.08                     | 0.52              |
| 35:DA:2105:C:C2'   | 35:DA:2106:G:H5'   | 2.39                     | 0.52              |
| 35:DA:252:G:O2'    | 35:DA:253:C:H5'    | 2.09                     | 0.52              |
| 35:DA:2873:A:H4'   | 50:DR:8:ARG:NH2    | 2.25                     | 0.52              |
| 35:DA:483:A:H2'    | 35:DA:483:A:N3     | 2.25                     | 0.52              |
| 37:DC:117:THR:HG22 | 37:DC:147:GLY:O    | 2.09                     | 0.52              |
| 40:DF:66:PRO:O     | 40:DF:67:GLN:HB3   | 2.09                     | 0.52              |
| 41:DG:133:LEU:CD1  | 41:DG:157:ILE:HB   | 2.30                     | 0.52              |
| 41:DG:94:LEU:HD22  | 41:DG:98:ARG:CB    | 2.39                     | 0.52              |
| 44:DK:106:GLU:CA   | 44:DK:109:LYS:HD3  | 2.30                     | 0.52              |
| 44:DK:17:ALA:HB3   | 44:DK:38:VAL:CG2   | 2.38                     | 0.52              |
| 46:DN:87:LEU:O     | 46:DN:90:MET:N     | 2.43                     | 0.52              |
| 48:DP:62:LEU:H     | 48:DP:62:LEU:HD22  | 1.75                     | 0.52              |
| 53:DU:79:PHE:CE2   | 53:DU:83:LEU:HD11  | 2.45                     | 0.52              |
| 58:DZ:18:LEU:O     | 58:DZ:21:ALA:HB3   | 2.10                     | 0.52              |
| 58:DZ:17:ALA:O     | 58:DZ:20:ARG:HG2   | 2.09                     | 0.52              |
| 1:AA:1131:G:C6     | 1:AA:1132:C:N4     | 2.79                     | 0.51              |
| 1:AA:1152:A:OP1    | 10:AJ:68:HIS:CD2   | 2.63                     | 0.51              |
| 1:AA:1287:A:H2'    | 1:AA:1288:A:C8     | 2.45                     | 0.51              |
| 1:AA:1512:U:H2'    | 1:AA:1513:A:C8     | 2.45                     | 0.51              |
| 1:AA:59:A:H3'      | 1:AA:331:G:H22     | 1.75                     | 0.51              |
| 2:AB:121:LEU:HA    | 2:AB:124:SER:HB3   | 1.91                     | 0.51              |
| 4:AD:159:ARG:O     | 4:AD:163:GLU:N     | 2.43                     | 0.51              |
| 1:AA:1152:A:OP1    | 10:AJ:68:HIS:HD2   | 1.93                     | 0.51              |
| 12:AL:27:LEU:C     | 12:AL:29:GLY:N     | 2.62                     | 0.51              |
| 12:AL:97:ARG:C     | 12:AL:98:TYR:CD1   | 2.83                     | 0.51              |
| 24:AY:205:TYR:O    | 24:AY:207:ASP:N    | 2.43                     | 0.51              |
| 24:AY:486:THR:HG21 | 24:AY:602:LEU:HD11 | 1.92                     | 0.51              |
| 30:B5:40:LYS:HZ1   | 30:B5:46:CYS:H     | 1.57                     | 0.51              |
| 31:B6:15:GLU:OE1   | 31:B6:41:PRO:CG    | 2.58                     | 0.51              |
| 35:BA:1465:G:H2'   | 35:BA:1466:G:H8    | 1.75                     | 0.51              |
| 35:BA:154(A):C:N4  | 35:BA:172:C:H42    | 2.07                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:1887:C:C3'   | 35:BA:1888:G:H5''  | 2.39                     | 0.51              |
| 35:BA:2543:G:H8    | 35:BA:2543:G:H5'   | 1.75                     | 0.51              |
| 35:BA:2811:G:O2'   | 35:BA:2812:G:H5'   | 2.10                     | 0.51              |
| 35:BA:302:C:H2'    | 35:BA:303:U:C6     | 2.45                     | 0.51              |
| 35:BA:272(I):U:C4  | 35:BA:363(A):A:N1  | 2.74                     | 0.51              |
| 35:BA:445:C:O2'    | 35:BA:446:G:H5'    | 2.09                     | 0.51              |
| 35:BA:860:U:O4'    | 35:BA:860:U:O2     | 2.28                     | 0.51              |
| 38:BD:26:LYS:HE2   | 38:BD:26:LYS:HA    | 1.91                     | 0.51              |
| 39:BE:116:VAL:HG22 | 39:BE:122:PHE:CG   | 2.46                     | 0.51              |
| 35:BA:2810:A:H2'   | 39:BE:61:ARG:HH21  | 1.74                     | 0.51              |
| 41:BG:146:TYR:O    | 41:BG:149:VAL:HG12 | 2.09                     | 0.51              |
| 41:BG:163:ALA:HB1  | 41:BG:168:GLU:HB2  | 1.91                     | 0.51              |
| 41:BG:77:ILE:HG21  | 41:BG:80:PHE:CB    | 2.40                     | 0.51              |
| 42:BH:104:GLU:HA   | 42:BH:113:VAL:O    | 2.10                     | 0.51              |
| 46:BN:10:GLU:CD    | 46:BN:11:PRO:HD2   | 2.31                     | 0.51              |
| 48:BP:13:ASN:O     | 48:BP:14:LYS:CB    | 2.58                     | 0.51              |
| 48:BP:47:ASP:HB3   | 48:BP:48:PRO:O     | 2.09                     | 0.51              |
| 49:BQ:2:LEU:O      | 49:BQ:3:MET:HB3    | 2.09                     | 0.51              |
| 49:BQ:69:PHE:CD1   | 49:BQ:70:PRO:HD2   | 2.44                     | 0.51              |
| 50:BR:104:ARG:HG3  | 50:BR:111:LEU:HD21 | 1.91                     | 0.51              |
| 50:BR:99:LYS:CD    | 50:BR:99:LYS:N     | 2.59                     | 0.51              |
| 53:BU:57:PHE:C     | 53:BU:59:ARG:N     | 2.62                     | 0.51              |
| 55:BW:36:LEU:HD12  | 55:BW:48:ALA:HA    | 1.92                     | 0.51              |
| 1:CA:117:G:O5'     | 1:CA:117:G:H8      | 1.92                     | 0.51              |
| 1:CA:346:G:H2'     | 1:CA:347:G:O4'     | 2.10                     | 0.51              |
| 1:CA:433:C:O2'     | 1:CA:434:U:H5'     | 2.10                     | 0.51              |
| 1:CA:512:U:H2'     | 1:CA:513:C:C6      | 2.45                     | 0.51              |
| 3:CC:134:ILE:O     | 3:CC:137:ALA:N     | 2.43                     | 0.51              |
| 3:CC:173:VAL:N     | 3:CC:174:PRO:HD3   | 2.25                     | 0.51              |
| 6:CF:3:ARG:HH11    | 6:CF:3:ARG:HG3     | 1.75                     | 0.51              |
| 9:CI:73:GLN:O      | 9:CI:76:ALA:N      | 2.44                     | 0.51              |
| 10:CJ:27:ALA:HB2   | 10:CJ:85:LEU:HD11  | 1.92                     | 0.51              |
| 18:CR:66:LEU:HG    | 18:CR:70:ILE:HD11  | 1.91                     | 0.51              |
| 24:CY:427:ALA:HB1  | 24:CY:466:LEU:CG   | 2.40                     | 0.51              |
| 24:CY:533:VAL:HG12 | 24:CY:571:SER:HA   | 1.92                     | 0.51              |
| 24:CY:549:ALA:HB2  | 24:CY:587:SER:OG   | 2.09                     | 0.51              |
| 29:D4:22:ILE:HD12  | 29:D4:22:ILE:N     | 2.25                     | 0.51              |
| 35:DA:1164:G:H1    | 35:DA:1185:C:H42   | 1.57                     | 0.51              |
| 35:DA:1192:G:H2'   | 35:DA:1193:G:O4'   | 2.10                     | 0.51              |
| 35:DA:1310:G:H2'   | 35:DA:1311:G:H5'   | 1.92                     | 0.51              |
| 35:DA:1400:G:H2'   | 35:DA:1401:G:C8    | 2.45                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:DA:2050:C:O2'  | 35:DA:2051:A:H5'   | 2.10                     | 0.51              |
| 35:DA:2296:U:C4'  | 35:DA:2297:C:OP1   | 2.52                     | 0.51              |
| 35:DA:278:A:C2    | 35:DA:279:C:C2     | 2.98                     | 0.51              |
| 35:DA:303:U:H2'   | 35:DA:304:G:H8     | 1.74                     | 0.51              |
| 35:DA:634:C:H2'   | 35:DA:635:C:C6     | 2.45                     | 0.51              |
| 36:DB:35:U:O2     | 36:DB:35:U:H2'     | 2.08                     | 0.51              |
| 36:DB:87:G:O3'    | 36:DB:88:C:C6      | 2.63                     | 0.51              |
| 38:DD:28:GLU:H    | 38:DD:29:PRO:HD2   | 1.75                     | 0.51              |
| 35:DA:2810:A:H2'  | 39:DE:61:ARG:HH21  | 1.74                     | 0.51              |
| 42:DH:54:ARG:O    | 42:DH:54:ARG:HD2   | 2.10                     | 0.51              |
| 42:DH:97:ARG:O    | 42:DH:98:LEU:C     | 2.47                     | 0.51              |
| 35:DA:1058:G:H21  | 44:DK:126:MET:CE   | 2.23                     | 0.51              |
| 44:DK:17:ALA:HB1  | 44:DK:38:VAL:HG22  | 1.92                     | 0.51              |
| 47:DO:113:LYS:O   | 47:DO:117:LEU:HD12 | 2.10                     | 0.51              |
| 47:DO:64:ARG:HH21 | 47:DO:100:GLY:HA3  | 1.75                     | 0.51              |
| 52:DT:50:ILE:HA   | 52:DT:99:LEU:CD1   | 2.40                     | 0.51              |
| 53:DU:10:ARG:O    | 53:DU:12:ARG:N     | 2.43                     | 0.51              |
| 55:DW:80:PRO:O    | 55:DW:100:THR:HG21 | 2.10                     | 0.51              |
| 1:AA:665:A:H2'    | 1:AA:732:C:O2      | 2.11                     | 0.51              |
| 3:AC:90:GLU:HA    | 3:AC:93:LYS:HB3    | 1.92                     | 0.51              |
| 4:AD:129:ASN:N    | 4:AD:129:ASN:HD22  | 2.07                     | 0.51              |
| 4:AD:150:GLU:HG2  | 4:AD:151:LYS:N     | 2.24                     | 0.51              |
| 4:AD:153:ARG:HG2  | 4:AD:153:ARG:NH1   | 2.25                     | 0.51              |
| 11:AK:29:ILE:HB   | 11:AK:44:SER:HB2   | 1.92                     | 0.51              |
| 16:AP:60:LEU:HD21 | 16:AP:66:PRO:HD3   | 1.92                     | 0.51              |
| 19:AS:27:GLU:O    | 19:AS:28:LYS:O     | 2.28                     | 0.51              |
| 22:AV:52:G:C2     | 22:AV:53:G:C8      | 2.99                     | 0.51              |
| 24:AY:9:LEU:O     | 24:AY:11:ARG:N     | 2.44                     | 0.51              |
| 24:AY:644:ARG:O   | 24:AY:645:ALA:HB2  | 2.10                     | 0.51              |
| 24:AY:688:ILE:O   | 24:AY:688:ILE:HG22 | 2.10                     | 0.51              |
| 31:B6:31:PRO:O    | 31:B6:32:ASN:OD1   | 2.28                     | 0.51              |
| 31:B6:10:LEU:HD12 | 33:B8:34:TRP:HB2   | 1.93                     | 0.51              |
| 35:BA:1145:C:H2'  | 35:BA:1146:C:H6    | 1.75                     | 0.51              |
| 35:BA:1231:G:H2'  | 35:BA:1232:G:C8    | 2.43                     | 0.51              |
| 35:BA:1721:G:H8   | 35:BA:1741:A:H62   | 1.58                     | 0.51              |
| 35:BA:2199:A:H3'  | 35:BA:2200:C:C6    | 2.46                     | 0.51              |
| 35:BA:2373:G:O2'  | 35:BA:2374:C:H5'   | 2.10                     | 0.51              |
| 31:B6:54:ILE:HD13 | 35:BA:2420:C:H5'   | 1.92                     | 0.51              |
| 35:BA:750:A:H3'   | 35:BA:751:A:H5''   | 1.92                     | 0.51              |
| 35:BA:841:A:H8    | 35:BA:841:A:H5'    | 1.75                     | 0.51              |
| 35:BA:943:U:OP2   | 48:BP:38:GLN:CD    | 2.48                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:BB:60:C:H2'    | 36:BB:61:G:C8      | 2.41                     | 0.51              |
| 38:BD:134:ARG:HG2 | 38:BD:187:GLY:O    | 2.11                     | 0.51              |
| 35:BA:2572:A:C8   | 39:BE:144:ARG:HB3  | 2.45                     | 0.51              |
| 39:BE:63:LEU:O    | 39:BE:64:LYS:C     | 2.48                     | 0.51              |
| 40:BF:69:HIS:N    | 40:BF:69:HIS:CD2   | 2.78                     | 0.51              |
| 41:BG:51:ARG:HA   | 41:BG:51:ARG:HE    | 1.74                     | 0.51              |
| 42:BH:140:LYS:O   | 42:BH:144:VAL:HG23 | 2.10                     | 0.51              |
| 42:BH:44:VAL:HG12 | 42:BH:45:VAL:H     | 1.75                     | 0.51              |
| 44:BK:84:LEU:HD21 | 44:BK:96:VAL:HB    | 1.91                     | 0.51              |
| 47:BO:111:PHE:O   | 47:BO:115:VAL:HG23 | 2.10                     | 0.51              |
| 52:BT:128:GLU:O   | 52:BT:129:ARG:HD3  | 2.11                     | 0.51              |
| 54:BV:25:LEU:H    | 54:BV:92:THR:HG21  | 1.74                     | 0.51              |
| 56:BX:12:VAL:HG12 | 56:BX:27:THR:C     | 2.31                     | 0.51              |
| 57:BY:28:LYS:HE3  | 57:BY:30:VAL:HG22  | 1.92                     | 0.51              |
| 1:CA:1058:G:H2'   | 1:CA:1059:C:C6     | 2.44                     | 0.51              |
| 1:CA:111:G:O6     | 1:CA:330:C:N4      | 2.42                     | 0.51              |
| 1:CA:1313:U:OP2   | 19:CS:6:LYS:CB     | 2.58                     | 0.51              |
| 1:CA:1394:A:N6    | 1:CA:1501:C:H5'    | 2.26                     | 0.51              |
| 1:CA:1478:C:O2'   | 1:CA:1479:C:H5'    | 2.10                     | 0.51              |
| 1:CA:539:A:H2'    | 1:CA:540:G:H8      | 1.74                     | 0.51              |
| 1:CA:814:A:H2'    | 1:CA:816:A:C5'     | 2.38                     | 0.51              |
| 6:CF:19:LEU:HD23  | 6:CF:19:LEU:C      | 2.30                     | 0.51              |
| 10:CJ:22:LYS:O    | 10:CJ:22:LYS:HD2   | 2.11                     | 0.51              |
| 10:CJ:3:LYS:HD2   | 10:CJ:77:PRO:CD    | 2.40                     | 0.51              |
| 1:CA:963:G:H21    | 10:CJ:55:LYS:CD    | 2.24                     | 0.51              |
| 10:CJ:8:LEU:HB2   | 10:CJ:70:ARG:O     | 2.09                     | 0.51              |
| 24:CY:125:ALA:C   | 24:CY:127:LYS:N    | 2.62                     | 0.51              |
| 24:CY:215:LYS:HA  | 24:CY:218:GLU:HB3  | 1.92                     | 0.51              |
| 24:CY:95:GLU:OE2  | 24:CY:124:GLN:HB3  | 2.11                     | 0.51              |
| 26:D1:53:VAL:CG2  | 26:D1:74:VAL:HG13  | 2.41                     | 0.51              |
| 26:D1:73:LEU:HD23 | 26:D1:73:LEU:O     | 2.11                     | 0.51              |
| 29:D4:10:VAL:CG2  | 29:D4:11:PRO:HD2   | 2.36                     | 0.51              |
| 31:D6:15:GLU:OE2  | 31:D6:44:ARG:CZ    | 2.57                     | 0.51              |
| 32:D7:48:LYS:NZ   | 35:DA:125:G:H21    | 2.06                     | 0.51              |
| 35:DA:1573:G:H2'  | 35:DA:1574:C:H5'   | 1.92                     | 0.51              |
| 35:DA:1683:C:H2'  | 35:DA:1684:C:H6    | 1.76                     | 0.51              |
| 35:DA:2377:A:O2'  | 35:DA:2378:A:H5'   | 2.09                     | 0.51              |
| 35:DA:2392:A:H2   | 35:DA:2424:C:H42   | 1.58                     | 0.51              |
| 35:DA:2422:A:H4'  | 35:DA:2423:U:OP1   | 2.10                     | 0.51              |
| 35:DA:402:A:O2'   | 35:DA:403:U:H5'    | 2.08                     | 0.51              |
| 36:DB:77:U:O2'    | 58:DZ:78:LYS:HE2   | 2.10                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:DC:30:VAL:O     | 37:DC:33:LEU:N     | 2.43                     | 0.51              |
| 35:DA:2050:C:H1'   | 39:DE:156:MET:CE   | 2.40                     | 0.51              |
| 39:DE:203:LYS:HG3  | 39:DE:204:ALA:N    | 2.25                     | 0.51              |
| 40:DF:168:ARG:C    | 40:DF:170:LEU:H    | 2.14                     | 0.51              |
| 41:DG:71:THR:CG2   | 41:DG:89:GLY:HA3   | 2.40                     | 0.51              |
| 53:DU:95:LEU:CD1   | 54:DV:11:GLN:HG3   | 2.39                     | 0.51              |
| 57:DY:43:ASN:HA    | 57:DY:64:GLU:HA    | 1.93                     | 0.51              |
| 57:DY:85:VAL:HG13  | 57:DY:93:GLY:O     | 2.10                     | 0.51              |
| 58:DZ:141:VAL:HG22 | 58:DZ:150:LEU:HD11 | 1.92                     | 0.51              |
| 49:DQ:55:VAL:HG23  | 58:DZ:178:GLU:HG3  | 1.91                     | 0.51              |
| 1:AA:1029:C:O2'    | 1:AA:1032:G:N2     | 2.43                     | 0.51              |
| 1:AA:1271:G:H2'    | 1:AA:1272:G:C8     | 2.45                     | 0.51              |
| 1:AA:1412:C:H2'    | 1:AA:1413:A:C8     | 2.45                     | 0.51              |
| 1:AA:439:A:H2'     | 1:AA:441:A:H5'     | 1.92                     | 0.51              |
| 1:AA:622:A:C8      | 1:AA:623:C:C5      | 2.98                     | 0.51              |
| 1:AA:779:C:O2'     | 11:AK:120:ARG:HD3  | 2.09                     | 0.51              |
| 2:AB:223:ILE:O     | 2:AB:225:ALA:N     | 2.44                     | 0.51              |
| 2:AB:84:GLU:HB3    | 2:AB:219:VAL:HG21  | 1.91                     | 0.51              |
| 4:AD:101:LEU:HD23  | 4:AD:121:VAL:HG13  | 1.92                     | 0.51              |
| 5:AE:36:ASP:O      | 5:AE:37:ARG:CB     | 2.58                     | 0.51              |
| 5:AE:60:TYR:HE1    | 5:AE:64:ARG:NH2    | 2.08                     | 0.51              |
| 11:AK:48:ILE:HG22  | 11:AK:49:GLY:N     | 2.25                     | 0.51              |
| 12:AL:39:VAL:HB    | 12:AL:57:LYS:HB2   | 1.91                     | 0.51              |
| 18:AR:40:LEU:C     | 18:AR:42:ARG:N     | 2.64                     | 0.51              |
| 19:AS:13:ASP:C     | 19:AS:15:LEU:N     | 2.63                     | 0.51              |
| 1:AA:263:A:OP2     | 20:AT:79:ARG:NH1   | 2.43                     | 0.51              |
| 22:AW:44:A:H2'     | 22:AW:45:A:C8      | 2.46                     | 0.51              |
| 24:AY:385:THR:HG21 | 24:AY:436:PRO:HG3  | 1.92                     | 0.51              |
| 12:AL:59:ARG:NE    | 24:AY:422:GLU:OE2  | 2.44                     | 0.51              |
| 24:AY:33:LEU:HD11  | 24:AY:81:ILE:HD12  | 1.93                     | 0.51              |
| 24:AY:15:ILE:CD1   | 24:AY:81:ILE:HG12  | 2.38                     | 0.51              |
| 26:B1:11:ARG:HB2   | 26:B1:12:PRO:HD2   | 1.92                     | 0.51              |
| 29:B4:51:ASP:OD2   | 29:B4:52:THR:N     | 2.43                     | 0.51              |
| 32:B7:17:GLY:O     | 32:B7:20:ALA:HB3   | 2.10                     | 0.51              |
| 33:B8:33:ASN:HA    | 33:B8:36:LYS:HG3   | 1.93                     | 0.51              |
| 33:B8:4:MET:HE1    | 33:B8:61:LEU:HD22  | 1.92                     | 0.51              |
| 35:BA:1161:C:H1'   | 54:BV:8:GLY:O      | 2.10                     | 0.51              |
| 35:BA:1516:C:C2'   | 35:BA:1517:G:C5'   | 2.88                     | 0.51              |
| 35:BA:2206:G:C2    | 35:BA:2207:G:H5'   | 2.45                     | 0.51              |
| 35:BA:2733:A:H2'   | 35:BA:2734:A:O4'   | 2.10                     | 0.51              |
| 35:BA:281:G:N2     | 35:BA:358:U:C5     | 2.79                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:537:C:H6     | 35:BA:537:C:O5'    | 1.93                     | 0.51              |
| 35:BA:648:G:H2'    | 35:BA:649:G:C8     | 2.44                     | 0.51              |
| 35:BA:664:C:O2'    | 35:BA:665:C:H5'    | 2.10                     | 0.51              |
| 37:BC:84:ILE:HG12  | 37:BC:96:GLY:O     | 2.10                     | 0.51              |
| 38:BD:248:SER:HB2  | 38:BD:249:PRO:HD2  | 1.92                     | 0.51              |
| 38:BD:28:GLU:H     | 38:BD:29:PRO:HD2   | 1.75                     | 0.51              |
| 39:BE:132:HIS:CD2  | 39:BE:135:HIS:NE2  | 2.78                     | 0.51              |
| 41:BG:63:ILE:HD12  | 41:BG:63:ILE:C     | 2.31                     | 0.51              |
| 42:BH:173:PRO:O    | 42:BH:175:LYS:N    | 2.43                     | 0.51              |
| 47:BO:60:ALA:C     | 47:BO:87:ILE:HD11  | 2.31                     | 0.51              |
| 48:BP:128:HIS:ND1  | 48:BP:148:LEU:HD13 | 2.25                     | 0.51              |
| 48:BP:38:GLN:CG    | 48:BP:39:LYS:H     | 2.07                     | 0.51              |
| 35:BA:389:G:N1     | 48:BP:71:VAL:HG12  | 2.23                     | 0.51              |
| 52:BT:55:ASN:H     | 52:BT:59:THR:HG21  | 1.76                     | 0.51              |
| 54:BV:13:ARG:HG3   | 54:BV:13:ARG:HH11  | 1.75                     | 0.51              |
| 1:CA:1365:G:O2'    | 1:CA:1366:C:H5'    | 2.09                     | 0.51              |
| 1:CA:1509:C:O2'    | 1:CA:1510:U:H5'    | 2.10                     | 0.51              |
| 2:CB:233:SER:OG    | 2:CB:234:PRO:HD2   | 2.10                     | 0.51              |
| 2:CB:51:LEU:CD2    | 2:CB:55:PHE:HE2    | 2.24                     | 0.51              |
| 4:CD:176:LEU:HD12  | 4:CD:177:ASP:N     | 2.25                     | 0.51              |
| 9:CI:79:LEU:HD11   | 9:CI:83:ARG:CD     | 2.40                     | 0.51              |
| 1:CA:1123:A:O3'    | 10:CJ:36:GLY:HA3   | 2.09                     | 0.51              |
| 1:CA:529:G:O6      | 12:CL:49:ASN:HA    | 2.10                     | 0.51              |
| 12:CL:39:VAL:HG21  | 12:CL:57:LYS:HD2   | 1.91                     | 0.51              |
| 13:CM:56:LEU:HD13  | 13:CM:60:VAL:HG23  | 1.92                     | 0.51              |
| 20:CT:57:ARG:HH11  | 20:CT:102:GLY:HA2  | 1.75                     | 0.51              |
| 24:CY:294:PRO:HG2  | 24:CY:295:GLU:OE2  | 2.11                     | 0.51              |
| 35:DA:1210:A:H5''  | 35:DA:1212:G:O4'   | 2.11                     | 0.51              |
| 35:DA:1829:A:N3    | 38:DD:15:PHE:CZ    | 2.78                     | 0.51              |
| 35:DA:2562:U:H1'   | 47:DO:23:ARG:NH1   | 2.19                     | 0.51              |
| 35:DA:2716:U:O2'   | 35:DA:2717:G:H5'   | 2.11                     | 0.51              |
| 35:DA:338:G:H2'    | 35:DA:339:U:C6     | 2.45                     | 0.51              |
| 35:DA:860:U:O2     | 35:DA:860:U:O4'    | 2.29                     | 0.51              |
| 37:DC:153:ILE:O    | 37:DC:157:ILE:HG13 | 2.11                     | 0.51              |
| 38:DD:78:LYS:HG2   | 38:DD:79:VAL:N     | 2.24                     | 0.51              |
| 40:DF:160:ASN:HD22 | 40:DF:161:GLU:N    | 2.07                     | 0.51              |
| 41:DG:181:ARG:NH1  | 41:DG:181:ARG:HB2  | 2.26                     | 0.51              |
| 35:DA:2308:G:H22   | 41:DG:79:ASN:HB2   | 1.73                     | 0.51              |
| 44:DK:112:MET:N    | 44:DK:113:PRO:CD   | 2.72                     | 0.51              |
| 48:DP:127:ALA:HB3  | 48:DP:130:PHE:CE1  | 2.45                     | 0.51              |
| 49:DQ:41:TRP:NE1   | 49:DQ:96:VAL:HG22  | 2.24                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 54:DV:13:ARG:HG3  | 54:DV:13:ARG:HH11  | 1.74                     | 0.51              |
| 54:DV:5:VAL:HG23  | 54:DV:37:VAL:HG23  | 1.91                     | 0.51              |
| 55:DW:9:TYR:H     | 55:DW:102:HIS:CD2  | 2.28                     | 0.51              |
| 57:DY:97:ARG:NH1  | 57:DY:97:ARG:HG3   | 2.24                     | 0.51              |
| 1:AA:1014:A:H5''  | 19:AS:14:HIS:HB2   | 1.92                     | 0.51              |
| 2:AB:137:ARG:HD3  | 2:AB:137:ARG:C     | 2.30                     | 0.51              |
| 3:AC:15:THR:HG21  | 3:AC:181:ASN:HA    | 1.91                     | 0.51              |
| 4:AD:119:GLN:HG3  | 4:AD:123:HIS:CD2   | 2.45                     | 0.51              |
| 19:AS:24:ALA:O    | 19:AS:25:LYS:CB    | 2.58                     | 0.51              |
| 22:AW:63:C:H2'    | 22:AW:64:G:C8      | 2.45                     | 0.51              |
| 26:B1:76:ARG:HH22 | 26:B1:95:LEU:CD2   | 2.24                     | 0.51              |
| 35:BA:1782:C:H2'  | 35:BA:1783:A:H5'   | 1.92                     | 0.51              |
| 35:BA:828:U:C5    | 35:BA:829:A:N6     | 2.79                     | 0.51              |
| 36:BB:87:G:O3'    | 36:BB:88:C:C6      | 2.63                     | 0.51              |
| 35:BA:2177:C:O2   | 37:BC:173:HIS:HE1  | 1.92                     | 0.51              |
| 38:BD:153:ALA:O   | 38:BD:154:LYS:CG   | 2.58                     | 0.51              |
| 39:BE:34:VAL:HG12 | 39:BE:48:GLN:O     | 2.10                     | 0.51              |
| 39:BE:69:LYS:O    | 39:BE:70:ALA:C     | 2.48                     | 0.51              |
| 41:BG:77:ILE:CG2  | 41:BG:80:PHE:N     | 2.62                     | 0.51              |
| 45:BL:87:UNK:HA   | 45:BL:90:UNK:CB    | 2.40                     | 0.51              |
| 46:BN:35:ARG:HB3  | 46:BN:42:TRP:CH2   | 2.45                     | 0.51              |
| 35:BA:941:A:H4'   | 48:BP:35:HIS:CE1   | 2.45                     | 0.51              |
| 30:B5:44:THR:HG23 | 50:BR:101:ALA:N    | 2.25                     | 0.51              |
| 52:BT:62:THR:HG22 | 52:BT:75:ILE:HG13  | 1.92                     | 0.51              |
| 54:BV:19:LYS:NZ   | 54:BV:22:VAL:HG13  | 2.26                     | 0.51              |
| 58:BZ:142:SER:H   | 58:BZ:144:LEU:CD2  | 2.21                     | 0.51              |
| 1:CA:1026:G:C3'   | 1:CA:1027:C:H5'    | 2.40                     | 0.51              |
| 1:CA:636:U:H2'    | 1:CA:637:G:C8      | 2.45                     | 0.51              |
| 1:CA:769:G:H4'    | 1:CA:1513:A:H4'    | 1.92                     | 0.51              |
| 3:CC:179:ARG:NH2  | 3:CC:206:GLU:OE2   | 2.43                     | 0.51              |
| 3:CC:32:LEU:O     | 3:CC:35:GLU:HB3    | 2.10                     | 0.51              |
| 6:CF:67:MET:HE1   | 6:CF:72:VAL:HA     | 1.92                     | 0.51              |
| 10:CJ:51:ARG:H    | 10:CJ:60:ARG:HA    | 1.75                     | 0.51              |
| 12:CL:78:GLN:O    | 12:CL:79:GLU:C     | 2.47                     | 0.51              |
| 13:CM:54:VAL:HG12 | 13:CM:58:GLU:HG2   | 1.91                     | 0.51              |
| 19:CS:79:THR:HG22 | 19:CS:80:TYR:N     | 2.25                     | 0.51              |
| 22:CW:5:G:O6      | 22:CW:69:C:N3      | 2.43                     | 0.51              |
| 24:CY:110:SER:HA  | 24:CY:149:VAL:HG21 | 1.93                     | 0.51              |
| 24:CY:153:MET:HA  | 24:CY:157:LEU:CD2  | 2.30                     | 0.51              |
| 24:CY:553:GLY:H   | 24:CY:557:GLY:CA   | 2.24                     | 0.51              |
| 24:CY:558:PHE:O   | 24:CY:559:PRO:C    | 2.49                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:CY:606:MET:HE3 | 24:CY:671:MET:HG2  | 1.92                     | 0.51              |
| 24:CY:90:PHE:HD1  | 24:CY:90:PHE:H     | 1.59                     | 0.51              |
| 28:D3:2:PRO:O     | 28:D3:3:ARG:O      | 2.29                     | 0.51              |
| 29:D4:19:GLY:O    | 29:D4:20:ASN:C     | 2.49                     | 0.51              |
| 35:DA:1576:U:H2'  | 35:DA:1577:C:C6    | 2.46                     | 0.51              |
| 35:DA:1596:A:O2'  | 35:DA:1597:A:H5'   | 2.10                     | 0.51              |
| 35:DA:1654:A:OP2  | 50:DR:3:HIS:HB2    | 2.10                     | 0.51              |
| 35:DA:1721:G:H8   | 35:DA:1741:A:H62   | 1.58                     | 0.51              |
| 35:DA:1947:C:H2'  | 35:DA:1948:G:C5'   | 2.36                     | 0.51              |
| 35:DA:2307:G:H21  | 35:DA:2308:G:C5'   | 2.23                     | 0.51              |
| 35:DA:260:G:H1'   | 35:DA:621:A:H1'    | 1.92                     | 0.51              |
| 35:DA:2626:C:H2'  | 35:DA:2627:G:O4'   | 2.10                     | 0.51              |
| 35:DA:272(I):U:O2 | 35:DA:272(I):U:C3' | 2.59                     | 0.51              |
| 35:DA:2820:A:O3'  | 50:DR:5:LYS:HE3    | 2.11                     | 0.51              |
| 35:DA:613:G:C8    | 35:DA:613:G:H5'    | 2.44                     | 0.51              |
| 35:DA:680:G:H2'   | 35:DA:681:G:H8     | 1.75                     | 0.51              |
| 35:DA:7:G:O2'     | 35:DA:8:A:H5'      | 2.11                     | 0.51              |
| 36:DB:94:C:H2'    | 36:DB:95:C:H6      | 1.75                     | 0.51              |
| 37:DC:73:VAL:CG1  | 37:DC:158:LYS:HA   | 2.39                     | 0.51              |
| 38:DD:210:GLY:O   | 38:DD:211:ARG:HB3  | 2.11                     | 0.51              |
| 39:DE:34:VAL:O    | 39:DE:34:VAL:HG22  | 2.11                     | 0.51              |
| 39:DE:38:THR:O    | 39:DE:42:ASP:HB2   | 2.11                     | 0.51              |
| 40:DF:24:LEU:O    | 40:DF:26:ALA:N     | 2.42                     | 0.51              |
| 41:DG:58:GLN:O    | 41:DG:61:ALA:HB3   | 2.10                     | 0.51              |
| 41:DG:57:ALA:HA   | 41:DG:90:LEU:CD2   | 2.41                     | 0.51              |
| 47:DO:20:MET:HE3  | 47:DO:44:LYS:HE3   | 1.93                     | 0.51              |
| 50:DR:104:ARG:HG3 | 50:DR:111:LEU:HD21 | 1.91                     | 0.51              |
| 54:DV:19:LYS:NZ   | 54:DV:22:VAL:HG13  | 2.25                     | 0.51              |
| 54:DV:62:LEU:N    | 54:DV:62:LEU:HD22  | 2.25                     | 0.51              |
| 56:DX:61:GLY:HA3  | 56:DX:73:ARG:O     | 2.10                     | 0.51              |
| 57:DY:95:LYS:CD   | 57:DY:101:LYS:H    | 2.24                     | 0.51              |
| 57:DY:14:LEU:HD11 | 57:DY:22:GLY:HA2   | 1.92                     | 0.51              |
| 58:DZ:10:ARG:HD2  | 58:DZ:36:LYS:CE    | 2.25                     | 0.51              |
| 1:AA:1149:C:H2'   | 1:AA:1150:U:C6     | 2.46                     | 0.51              |
| 1:AA:117:G:H8     | 1:AA:117:G:O5'     | 1.94                     | 0.51              |
| 1:AA:119:A:O2'    | 1:AA:120:A:OP2     | 2.19                     | 0.51              |
| 1:AA:1237:C:OP1   | 1:AA:1238:A:H1'    | 2.10                     | 0.51              |
| 8:AH:114:THR:HG21 | 8:AH:129:VAL:HG23  | 1.93                     | 0.51              |
| 13:AM:96:LEU:HB3  | 13:AM:97:PRO:CD    | 2.33                     | 0.51              |
| 17:AQ:40:LYS:HD3  | 17:AQ:42:TYR:OH    | 2.11                     | 0.51              |
| 20:AT:26:ASN:HB3  | 20:AT:71:THR:OG1   | 2.10                     | 0.51              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:AW:18:U:O2      | 22:AW:18:U:H2'     | 2.10                     | 0.51              |
| 24:AY:350:GLU:HA   | 24:AY:350:GLU:OE1  | 2.10                     | 0.51              |
| 24:AY:428:LEU:HD13 | 24:AY:440:VAL:CG1  | 2.28                     | 0.51              |
| 24:AY:603:GLU:HB2  | 24:AY:604:PRO:HD2  | 1.91                     | 0.51              |
| 24:AY:65:ILE:O     | 24:AY:67:ALA:N     | 2.44                     | 0.51              |
| 30:B5:55:ARG:O     | 30:B5:56:LYS:CB    | 2.51                     | 0.51              |
| 31:B6:54:ILE:HD13  | 35:BA:2420:C:C4'   | 2.39                     | 0.51              |
| 33:B8:53:PRO:HA    | 33:B8:56:GLU:HB2   | 1.93                     | 0.51              |
| 35:BA:1047:G:HO2'  | 35:BA:1110:G:N2    | 2.09                     | 0.51              |
| 35:BA:1230:C:H2'   | 35:BA:1231:G:C8    | 2.45                     | 0.51              |
| 35:BA:1528:A:C2    | 35:BA:1542:A:H2    | 2.29                     | 0.51              |
| 35:BA:1858:G:H2'   | 35:BA:1883:G:N2    | 2.25                     | 0.51              |
| 35:BA:2859:G:H2'   | 35:BA:2860:A:C8    | 2.46                     | 0.51              |
| 35:BA:787:U:OP1    | 35:BA:1780:A:N6    | 2.43                     | 0.51              |
| 35:BA:852:G:H2'    | 35:BA:853:G:C8     | 2.45                     | 0.51              |
| 44:BK:70:LYS:HE3   | 44:BK:70:LYS:N     | 2.26                     | 0.51              |
| 51:BS:101:LEU:C    | 51:BS:101:LEU:HD12 | 2.31                     | 0.51              |
| 52:BT:112:ARG:C    | 52:BT:115:ARG:HD3  | 2.31                     | 0.51              |
| 52:BT:99:LEU:HB2   | 52:BT:101:PHE:CE1  | 2.46                     | 0.51              |
| 53:BU:61:TRP:CB    | 53:BU:93:LYS:HB3   | 2.39                     | 0.51              |
| 53:BU:92:ARG:HD3   | 53:BU:94:ASN:CB    | 2.41                     | 0.51              |
| 54:BV:16:PRO:O     | 54:BV:96:ILE:O     | 2.28                     | 0.51              |
| 57:BY:14:LEU:HD11  | 57:BY:22:GLY:HA2   | 1.93                     | 0.51              |
| 57:BY:94:LYS:O     | 57:BY:102:CYS:HB2  | 2.10                     | 0.51              |
| 1:CA:1129:C:H5'    | 1:CA:1129:C:H6     | 1.75                     | 0.51              |
| 1:CA:1360:A:H2'    | 1:CA:1361:G:O4'    | 2.11                     | 0.51              |
| 1:CA:375:U:C2      | 1:CA:376:G:C8      | 2.98                     | 0.51              |
| 1:CA:986:A:H2'     | 1:CA:987:G:C8      | 2.46                     | 0.51              |
| 2:CB:151:GLY:O     | 2:CB:152:PHE:C     | 2.48                     | 0.51              |
| 4:CD:96:LEU:N      | 4:CD:96:LEU:HD22   | 2.23                     | 0.51              |
| 5:CE:51:VAL:HB     | 5:CE:52:PRO:CD     | 2.41                     | 0.51              |
| 6:CF:72:VAL:HG13   | 6:CF:73:ASN:N      | 2.26                     | 0.51              |
| 1:CA:1345:U:OP1    | 9:CI:120:ARG:NH1   | 2.43                     | 0.51              |
| 10:CJ:3:LYS:HG3    | 10:CJ:75:ILE:O     | 2.10                     | 0.51              |
| 13:CM:91:ARG:HH21  | 19:CS:81:ARG:HH21  | 1.57                     | 0.51              |
| 16:CP:8:ARG:NH2    | 16:CP:15:PRO:HG3   | 2.26                     | 0.51              |
| 17:CQ:59:ILE:HG23  | 17:CQ:71:PHE:CB    | 2.34                     | 0.51              |
| 24:CY:335:LEU:O    | 24:CY:368:GLU:HA   | 2.09                     | 0.51              |
| 24:CY:394:ALA:HB1  | 24:CY:395:PRO:CD   | 2.41                     | 0.51              |
| 24:CY:544:LYS:O    | 24:CY:548:GLU:HB3  | 2.10                     | 0.51              |
| 31:D6:9:LEU:CD2    | 31:D6:26:ASN:HD22  | 2.24                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 31:D6:42:TRP:HA     | 31:D6:42:TRP:CE3   | 2.44                     | 0.51              |
| 35:DA:1820:U:C2     | 38:DD:202:LYS:HG2  | 2.45                     | 0.51              |
| 35:DA:528:A:H2      | 35:DA:2043:C:H5'   | 1.74                     | 0.51              |
| 35:DA:211:A:C3'     | 35:DA:212:G:H5''   | 2.40                     | 0.51              |
| 35:DA:2577:A:H5'    | 35:DA:2578:G:C5'   | 2.39                     | 0.51              |
| 35:DA:2776:A:H4'    | 35:DA:2777:G:H5''  | 1.93                     | 0.51              |
| 35:DA:2784:C:H1'    | 39:DE:37:ARG:HH12  | 1.75                     | 0.51              |
| 35:DA:2860:A:C2'    | 35:DA:2861:G:H5'   | 2.40                     | 0.51              |
| 35:DA:588:U:H1'     | 40:DF:90:PHE:CG    | 2.45                     | 0.51              |
| 35:DA:796:C:H2'     | 35:DA:797:C:H6     | 1.73                     | 0.51              |
| 37:DC:98:GLU:O      | 37:DC:101:ILE:HD13 | 2.10                     | 0.51              |
| 35:DA:782:A:C2      | 38:DD:226:MET:HG2  | 2.46                     | 0.51              |
| 42:DH:34:GLU:O      | 42:DH:36:PRO:HD3   | 2.11                     | 0.51              |
| 46:DN:23:LEU:HB3    | 46:DN:60:ILE:CG2   | 2.37                     | 0.51              |
| 49:DQ:108:GLY:O     | 49:DQ:109:VAL:HG23 | 2.11                     | 0.51              |
| 49:DQ:109:VAL:HG12  | 49:DQ:110:THR:N    | 2.24                     | 0.51              |
| 35:DA:2870:C:H5''   | 50:DR:65:LEU:HD21  | 1.93                     | 0.51              |
| 50:DR:72:ASP:CG     | 50:DR:75:LEU:H     | 2.14                     | 0.51              |
| 35:DA:1248:G:C4     | 53:DU:3:ARG:HD2    | 2.45                     | 0.51              |
| 54:DV:49:THR:HB     | 54:DV:50:PRO:HD2   | 1.92                     | 0.51              |
| 55:DW:20:VAL:O      | 55:DW:23:LEU:N     | 2.42                     | 0.51              |
| 57:DY:12:THR:HG23   | 57:DY:25:GLY:O     | 2.11                     | 0.51              |
| 1:AA:1129:C:H6      | 1:AA:1129:C:H5'    | 1.74                     | 0.51              |
| 8:AH:104:ARG:O      | 8:AH:105:ARG:C     | 2.48                     | 0.51              |
| 9:AI:18:PHE:O       | 9:AI:61:ALA:HA     | 2.10                     | 0.51              |
| 9:AI:40:LEU:CD1     | 9:AI:70:LYS:HG2    | 2.40                     | 0.51              |
| 20:AT:42:GLN:NE2    | 20:AT:42:GLN:HA    | 2.25                     | 0.51              |
| 24:AY:216:LEU:HD23  | 24:AY:216:LEU:C    | 2.31                     | 0.51              |
| 25:B0:25:ARG:HD2    | 25:B0:29:GLN:HE21  | 1.73                     | 0.51              |
| 27:B2:48:HIS:CD2    | 35:BA:96:G:H4'     | 2.45                     | 0.51              |
| 31:B6:11:LEU:HD13   | 31:B6:11:LEU:O     | 2.11                     | 0.51              |
| 33:B8:15:LYS:HB2    | 48:BP:65:ARG:HH12  | 1.75                     | 0.51              |
| 35:BA:1035:U:H2'    | 35:BA:1036:G:C8    | 2.44                     | 0.51              |
| 35:BA:1450(A):C:H2' | 35:BA:1451:C:C6    | 2.45                     | 0.51              |
| 35:BA:1477:A:H5'    | 35:BA:1478:G:OP2   | 2.11                     | 0.51              |
| 35:BA:120:U:O2'     | 35:BA:149:A:C8     | 2.60                     | 0.51              |
| 35:BA:1899:G:O2'    | 35:BA:1900:A:H5''  | 2.11                     | 0.51              |
| 35:BA:1908:C:H2'    | 35:BA:1909:C:H6    | 1.75                     | 0.51              |
| 35:BA:2020:A:H2'    | 35:BA:2021:C:H5''  | 1.91                     | 0.51              |
| 35:BA:2220:G:H2'    | 35:BA:2221:G:H8    | 1.76                     | 0.51              |
| 35:BA:2377:A:O2'    | 35:BA:2378:A:H5'   | 2.10                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:2617:C:C2'   | 35:BA:2618:G:H5'   | 2.41                     | 0.51              |
| 35:BA:2872:G:C2    | 35:BA:2873:A:N6    | 2.78                     | 0.51              |
| 35:BA:338:G:H2'    | 35:BA:339:U:C6     | 2.46                     | 0.51              |
| 35:BA:536:A:H2'    | 35:BA:537:C:C6     | 2.46                     | 0.51              |
| 35:BA:685:A:C5     | 35:BA:774:A:C2     | 2.98                     | 0.51              |
| 37:BC:149:ASN:HD22 | 37:BC:149:ASN:N    | 2.07                     | 0.51              |
| 38:BD:134:ARG:HG3  | 38:BD:135:PHE:HD1  | 1.75                     | 0.51              |
| 38:BD:239:ARG:HH21 | 38:BD:239:ARG:HG2  | 1.75                     | 0.51              |
| 38:BD:9:TYR:CD2    | 38:BD:10:THR:HG22  | 2.45                     | 0.51              |
| 39:BE:116:VAL:O    | 39:BE:117:MET:CB   | 2.42                     | 0.51              |
| 39:BE:152:LYS:HG3  | 39:BE:153:GLY:N    | 2.26                     | 0.51              |
| 39:BE:104:VAL:HG22 | 39:BE:198:VAL:HG22 | 1.91                     | 0.51              |
| 40:BF:181:LEU:HB3  | 40:BF:205:ARG:HH12 | 1.69                     | 0.51              |
| 42:BH:103:LEU:HB2  | 42:BH:123:PHE:HD2  | 1.75                     | 0.51              |
| 46:BN:133:GLN:O    | 46:BN:134:ARG:HB3  | 2.11                     | 0.51              |
| 48:BP:146:VAL:HG13 | 48:BP:147:LEU:N    | 2.25                     | 0.51              |
| 53:BU:110:VAL:HG12 | 53:BU:114:LYS:HD2  | 1.91                     | 0.51              |
| 58:BZ:3:TYR:CD2    | 58:BZ:51:ALA:HB2   | 2.45                     | 0.51              |
| 1:CA:1073:U:O2'    | 1:CA:1074:G:H5'    | 2.11                     | 0.51              |
| 1:CA:1124:G:C5'    | 10:CJ:35:SER:HB2   | 2.41                     | 0.51              |
| 1:CA:119:A:O2'     | 1:CA:120:A:OP2     | 2.26                     | 0.51              |
| 1:CA:1378:C:OP1    | 7:CG:7:ALA:HB3     | 2.10                     | 0.51              |
| 1:CA:1512:U:H2'    | 1:CA:1513:A:C8     | 2.44                     | 0.51              |
| 1:CA:159:G:C2'     | 1:CA:160:A:H5''    | 2.41                     | 0.51              |
| 2:CB:97:TRP:CH2    | 2:CB:176:GLU:CD    | 2.84                     | 0.51              |
| 2:CB:236:TYR:HA    | 2:CB:239:VAL:HG23  | 1.93                     | 0.51              |
| 2:CB:84:GLU:HB3    | 2:CB:219:VAL:HG21  | 1.92                     | 0.51              |
| 2:CB:8:LYS:O       | 2:CB:11:LEU:N      | 2.39                     | 0.51              |
| 12:CL:26:ALA:O     | 12:CL:27:LEU:O     | 2.29                     | 0.51              |
| 22:CW:65:G:H2'     | 22:CW:66:C:O4'     | 2.11                     | 0.51              |
| 24:CY:165:GLN:HE21 | 24:CY:177:ILE:HG21 | 1.75                     | 0.51              |
| 24:CY:181:LEU:HD12 | 24:CY:242:LEU:HD13 | 1.93                     | 0.51              |
| 24:CY:510:VAL:HA   | 24:CY:570:GLY:CA   | 2.40                     | 0.51              |
| 28:D3:56:VAL:CG1   | 28:D3:57:GLU:N     | 2.74                     | 0.51              |
| 13:CM:3:ARG:HD3    | 29:D4:34:GLU:HG2   | 1.92                     | 0.51              |
| 34:D9:29:ASN:H     | 34:D9:29:ASN:ND2   | 2.09                     | 0.51              |
| 35:DA:990:A:C6     | 35:DA:1186:G:H1'   | 2.45                     | 0.51              |
| 35:DA:1515:G:H2'   | 35:DA:1516:C:C6    | 2.45                     | 0.51              |
| 35:DA:1517:G:C8    | 35:DA:1517:G:H5'   | 2.40                     | 0.51              |
| 35:DA:1748:G:H5'   | 35:DA:1748:G:C8    | 2.40                     | 0.51              |
| 35:DA:1999:C:O2'   | 35:DA:2000:G:H5'   | 2.10                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:208:C:H2'    | 35:DA:209:C:H6     | 1.74                     | 0.51              |
| 35:DA:2298:A:N6    | 35:DA:2318:G:H8    | 2.08                     | 0.51              |
| 35:DA:2465:C:O2'   | 35:DA:2466:C:H5'   | 2.11                     | 0.51              |
| 35:DA:2502:G:H5''  | 35:DA:2503:A:C5'   | 2.37                     | 0.51              |
| 35:DA:2747:G:H21   | 35:DA:2757:A:H62   | 1.58                     | 0.51              |
| 37:DC:104:ILE:HG23 | 37:DC:108:TRP:O    | 2.11                     | 0.51              |
| 38:DD:4:LYS:NZ     | 38:DD:21:PHE:H     | 2.09                     | 0.51              |
| 41:DG:103:LEU:HD23 | 41:DG:106:LEU:HD23 | 1.92                     | 0.51              |
| 41:DG:108:ASN:O    | 41:DG:109:VAL:HG23 | 2.10                     | 0.51              |
| 41:DG:59:GLU:HG2   | 41:DG:60:LEU:N     | 2.26                     | 0.51              |
| 46:DN:18:ALA:HB3   | 46:DN:21:LYS:HB2   | 1.92                     | 0.51              |
| 58:DZ:99:TYR:CE2   | 58:DZ:125:LEU:HB2  | 2.46                     | 0.51              |
| 1:AA:1118:C:OP1    | 9:AI:104:ARG:NH1   | 2.44                     | 0.51              |
| 1:AA:1122:U:C2'    | 1:AA:1123:A:H5'    | 2.40                     | 0.51              |
| 1:AA:1134:G:C2'    | 1:AA:1135:U:H5'    | 2.40                     | 0.51              |
| 1:AA:1294:G:C2'    | 1:AA:1295:G:H5'    | 2.41                     | 0.51              |
| 1:AA:460:G:O6      | 1:AA:470:C:H4'     | 2.11                     | 0.51              |
| 2:AB:236:TYR:HA    | 2:AB:239:VAL:HG23  | 1.92                     | 0.51              |
| 6:AF:38:GLU:HB2    | 6:AF:64:GLN:O      | 2.10                     | 0.51              |
| 7:AG:29:LYS:HB2    | 7:AG:105:VAL:HG21  | 1.93                     | 0.51              |
| 8:AH:29:SER:OG     | 8:AH:32:LYS:HG3    | 2.10                     | 0.51              |
| 9:AI:24:GLY:HA2    | 9:AI:59:PHE:O      | 2.10                     | 0.51              |
| 12:AL:41:ARG:HH11  | 12:AL:41:ARG:CB    | 2.19                     | 0.51              |
| 13:AM:54:VAL:O     | 13:AM:56:LEU:N     | 2.43                     | 0.51              |
| 19:AS:10:PHE:HZ    | 19:AS:70:LYS:HZ3   | 1.57                     | 0.51              |
| 23:AX:13:A:H5'     | 23:AX:14:A:OP2     | 2.11                     | 0.51              |
| 24:AY:282:SER:C    | 24:AY:284:LEU:H    | 2.14                     | 0.51              |
| 24:AY:367:GLU:O    | 24:AY:368:GLU:HB3  | 2.10                     | 0.51              |
| 24:AY:616:TYR:HB3  | 24:AY:662:LYS:O    | 2.11                     | 0.51              |
| 35:BA:1164:G:H1    | 35:BA:1185:C:H42   | 1.58                     | 0.51              |
| 35:BA:515:A:C2     | 35:BA:1261:C:H1'   | 2.46                     | 0.51              |
| 35:BA:1718:G:C8    | 35:BA:1718:G:H5'   | 2.43                     | 0.51              |
| 35:BA:1998:G:O2'   | 35:BA:1999:C:H5'   | 2.10                     | 0.51              |
| 35:BA:644:A:C2     | 35:BA:2369:A:H1'   | 2.46                     | 0.51              |
| 35:BA:274:G:C2'    | 35:BA:274:G:N3     | 2.74                     | 0.51              |
| 35:BA:567:A:N1     | 35:BA:571:A:H8     | 2.09                     | 0.51              |
| 38:BD:35:LYS:HG2   | 38:BD:63:ARG:HG3   | 1.92                     | 0.51              |
| 40:BF:160:ASN:ND2  | 40:BF:160:ASN:C    | 2.63                     | 0.51              |
| 40:BF:24:LEU:O     | 40:BF:26:ALA:N     | 2.43                     | 0.51              |
| 41:BG:82:LEU:C     | 41:BG:82:LEU:HD23  | 2.31                     | 0.51              |
| 42:BH:105:LEU:HD23 | 42:BH:105:LEU:N    | 2.25                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 42:BH:37:VAL:CG1    | 42:BH:38:SER:N     | 2.74                     | 0.51              |
| 46:BN:132:ALA:O     | 46:BN:133:GLN:HB2  | 2.11                     | 0.51              |
| 46:BN:137:LYS:O     | 46:BN:138:LEU:HD23 | 2.10                     | 0.51              |
| 48:BP:9:ASN:N       | 48:BP:10:PRO:CD    | 2.74                     | 0.51              |
| 35:BA:943:U:OP2     | 48:BP:38:GLN:OE1   | 2.28                     | 0.51              |
| 49:BQ:109:VAL:HG12  | 49:BQ:110:THR:N    | 2.25                     | 0.51              |
| 49:BQ:54:MET:CG     | 49:BQ:64:ILE:HD13  | 2.39                     | 0.51              |
| 51:BS:30:ARG:HH22   | 51:BS:62:LYS:HD2   | 1.75                     | 0.51              |
| 58:BZ:107:THR:HG23  | 58:BZ:111:VAL:CG2  | 2.40                     | 0.51              |
| 1:CA:771:G:H2'      | 1:CA:772:U:C6      | 2.45                     | 0.51              |
| 2:CB:54:THR:HG21    | 2:CB:201:ILE:HD11  | 1.93                     | 0.51              |
| 3:CC:136:GLN:C      | 3:CC:138:VAL:N     | 2.59                     | 0.51              |
| 4:CD:155:LEU:O      | 4:CD:156:GLU:C     | 2.49                     | 0.51              |
| 5:CE:78:HIS:CE1     | 5:CE:80:ILE:HG23   | 2.46                     | 0.51              |
| 6:CF:45:LEU:O       | 6:CF:46:ARG:CG     | 2.58                     | 0.51              |
| 6:CF:71:ARG:NH1     | 6:CF:71:ARG:HG3    | 2.25                     | 0.51              |
| 8:CH:83:ILE:CD1     | 8:CH:137:VAL:HG22  | 2.35                     | 0.51              |
| 11:CK:17:GLY:O      | 11:CK:80:VAL:HA    | 2.10                     | 0.51              |
| 1:CA:719:C:C2       | 18:CR:50:ILE:HG12  | 2.45                     | 0.51              |
| 24:CY:448:GLN:HE22  | 24:CY:480:GLN:HE21 | 1.59                     | 0.51              |
| 24:CY:609:GLU:HG3   | 24:CY:670:VAL:HG21 | 1.92                     | 0.51              |
| 27:D2:10:LEU:HD22   | 27:D2:14:ARG:NH2   | 2.26                     | 0.51              |
| 35:DA:1450(A):C:H2' | 35:DA:1451:C:C6    | 2.46                     | 0.51              |
| 35:DA:1913:A:H4'    | 35:DA:1914:C:H5''  | 1.91                     | 0.51              |
| 35:DA:2230:G:H2'    | 35:DA:2231:C:C6    | 2.46                     | 0.51              |
| 35:DA:2590:A:OP2    | 38:DD:238:GLY:HA2  | 2.11                     | 0.51              |
| 39:DE:1:MET:HB2     | 39:DE:83:ASP:O     | 2.10                     | 0.51              |
| 40:DF:174:VAL:HG21  | 40:DF:189:THR:CG2  | 2.41                     | 0.51              |
| 41:DG:105:LYS:HD3   | 41:DG:143:GLU:OE1  | 2.11                     | 0.51              |
| 42:DH:84:SER:OG     | 42:DH:85:LYS:N     | 2.43                     | 0.51              |
| 44:DK:70:LYS:HE3    | 44:DK:70:LYS:N     | 2.25                     | 0.51              |
| 46:DN:1:MET:HE2     | 46:DN:2:LYS:N      | 2.26                     | 0.51              |
| 46:DN:65:LYS:HZ2    | 46:DN:65:LYS:CB    | 2.20                     | 0.51              |
| 50:DR:12:ARG:HB3    | 50:DR:16:HIS:CD2   | 2.46                     | 0.51              |
| 52:DT:112:ARG:C     | 52:DT:115:ARG:HD3  | 2.31                     | 0.51              |
| 54:DV:19:LYS:HB3    | 54:DV:94:LEU:O     | 2.10                     | 0.51              |
| 1:AA:1452:C:H1'     | 1:AA:1456:G:C2     | 2.44                     | 0.51              |
| 1:AA:265:G:H2'      | 1:AA:267:C:H5      | 1.76                     | 0.51              |
| 1:AA:509:A:C2       | 1:AA:510:A:C2      | 2.98                     | 0.51              |
| 1:AA:703:G:O2'      | 1:AA:704:A:OP2     | 2.29                     | 0.51              |
| 1:AA:956:U:H2'      | 1:AA:957:U:H6      | 1.76                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:AB:97:TRP:HH2    | 2:AB:176:GLU:CD    | 2.13                     | 0.51              |
| 2:AB:51:LEU:HD23   | 2:AB:201:ILE:HD12  | 1.91                     | 0.51              |
| 3:AC:181:ASN:HD21  | 3:AC:204:LEU:HD12  | 1.75                     | 0.51              |
| 4:AD:12:CYS:SG     | 4:AD:19:LEU:O      | 2.69                     | 0.51              |
| 10:AJ:37:PRO:CA    | 10:AJ:72:VAL:HG22  | 2.36                     | 0.51              |
| 13:AM:9:ILE:HD12   | 13:AM:9:ILE:N      | 2.25                     | 0.51              |
| 15:AO:65:ARG:HD2   | 15:AO:65:ARG:H     | 1.76                     | 0.51              |
| 20:AT:48:LYS:HD2   | 20:AT:51:GLU:OE2   | 2.11                     | 0.51              |
| 20:AT:74:LYS:HD3   | 20:AT:74:LYS:H     | 1.76                     | 0.51              |
| 22:AV:73:A:O3'     | 22:AV:74:C:H6      | 1.94                     | 0.51              |
| 24:AY:122:TRP:CD1  | 24:AY:123:ARG:N    | 2.79                     | 0.51              |
| 24:AY:573:HIS:CD2  | 24:AY:575:VAL:H    | 2.28                     | 0.51              |
| 24:AY:616:TYR:CD2  | 24:AY:663:THR:HA   | 2.46                     | 0.51              |
| 24:AY:519:ARG:NH1  | 24:AY:678:GLU:CB   | 2.74                     | 0.51              |
| 31:B6:15:GLU:HB2   | 31:B6:49:HIS:CE1   | 2.45                     | 0.51              |
| 31:B6:11:LEU:CD2   | 31:B6:51:GLU:HG3   | 2.40                     | 0.51              |
| 35:BA:990:A:C6     | 35:BA:1186:G:H1'   | 2.45                     | 0.51              |
| 35:BA:1420:U:H2'   | 35:BA:1421:G:H5'   | 1.92                     | 0.51              |
| 31:B6:8:LYS:NZ     | 35:BA:2285:C:C5    | 2.77                     | 0.51              |
| 35:BA:2395:C:C2    | 35:BA:2396:G:C8    | 2.99                     | 0.51              |
| 35:BA:2771:C:H2'   | 35:BA:2772:C:C6    | 2.46                     | 0.51              |
| 35:BA:2875:C:O2'   | 52:BT:5:ALA:HB3    | 2.11                     | 0.51              |
| 35:BA:346:A:N3     | 35:BA:346:A:H2'    | 2.26                     | 0.51              |
| 35:BA:658:C:H2'    | 35:BA:659:C:C6     | 2.46                     | 0.51              |
| 35:BA:958:U:H6     | 35:BA:958:U:H3'    | 1.76                     | 0.51              |
| 38:BD:267:SER:C    | 38:BD:269:PHE:H    | 2.14                     | 0.51              |
| 46:BN:89:LYS:O     | 46:BN:93:THR:HG22  | 2.10                     | 0.51              |
| 52:BT:48:ILE:HD12  | 52:BT:48:ILE:N     | 2.25                     | 0.51              |
| 58:BZ:152:ALA:CA   | 58:BZ:167:PRO:HB2  | 2.41                     | 0.51              |
| 1:CA:1134:G:C2'    | 1:CA:1135:U:H5'    | 2.41                     | 0.51              |
| 1:CA:129(A):G:C6   | 1:CA:189(E):U:H4'  | 2.46                     | 0.51              |
| 1:CA:276:G:O2'     | 1:CA:277:C:H5'     | 2.10                     | 0.51              |
| 1:CA:59:A:H3'      | 1:CA:331:G:H22     | 1.75                     | 0.51              |
| 1:CA:771:G:H2'     | 1:CA:772:U:H6      | 1.76                     | 0.51              |
| 1:CA:980:C:H2'     | 1:CA:981:U:H5'     | 1.93                     | 0.51              |
| 10:CJ:4:ILE:HB     | 10:CJ:74:ILE:CD1   | 2.40                     | 0.51              |
| 10:CJ:78:ASN:C     | 10:CJ:79:ARG:HH11  | 2.15                     | 0.51              |
| 13:CM:119:GLY:O    | 13:CM:120:LYS:HB2  | 2.11                     | 0.51              |
| 13:CM:96:LEU:HB3   | 13:CM:97:PRO:CD    | 2.36                     | 0.51              |
| 24:CY:106:VAL:HG23 | 24:CY:132:ARG:HG3  | 1.93                     | 0.51              |
| 24:CY:162:VAL:HG11 | 24:CY:216:LEU:HD12 | 1.92                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:CY:68:ALA:HB3   | 24:CY:327:PHE:CE1 | 2.46                     | 0.51              |
| 31:D6:17:LYS:O     | 31:D6:20:ASN:ND2  | 2.44                     | 0.51              |
| 35:DA:86:C:H4'     | 35:DA:104:U:H1'   | 1.92                     | 0.51              |
| 35:DA:1063:G:O2'   | 35:DA:1064:C:H5'  | 2.10                     | 0.51              |
| 35:DA:1204:A:N1    | 35:DA:1241:A:H2   | 2.07                     | 0.51              |
| 35:DA:1719:G:C2'   | 35:DA:1720:U:H5'  | 2.40                     | 0.51              |
| 35:DA:802:A:H2'    | 35:DA:803:U:C6    | 2.45                     | 0.51              |
| 36:DB:94:C:H2'     | 36:DB:95:C:C6     | 2.46                     | 0.51              |
| 39:DE:116:VAL:O    | 39:DE:117:MET:CB  | 2.47                     | 0.51              |
| 39:DE:116:VAL:HG21 | 39:DE:122:PHE:CD2 | 2.45                     | 0.51              |
| 42:DH:46:GLU:HG3   | 42:DH:51:ARG:HB2  | 1.92                     | 0.51              |
| 46:DN:35:ARG:HB3   | 46:DN:42:TRP:CH2  | 2.46                     | 0.51              |
| 47:DO:34:THR:O     | 47:DO:35:VAL:C    | 2.49                     | 0.51              |
| 48:DP:47:ASP:OD1   | 48:DP:49:ARG:HB2  | 2.10                     | 0.51              |
| 49:DQ:75:THR:CG2   | 49:DQ:76:LYS:N    | 2.74                     | 0.51              |
| 53:DU:79:PHE:O     | 53:DU:83:LEU:HD13 | 2.11                     | 0.51              |
| 54:DV:35:LEU:C     | 54:DV:37:VAL:N    | 2.63                     | 0.51              |
| 27:D2:37:PHE:HE2   | 56:DX:11:PRO:HB3  | 1.76                     | 0.51              |
| 57:DY:10:GLY:O     | 57:DY:27:VAL:HG22 | 2.10                     | 0.51              |
| 58:DZ:179:ASP:HB3  | 58:DZ:182:LYS:CE  | 2.29                     | 0.51              |
| 58:DZ:185:GLU:O    | 58:DZ:187:ALA:N   | 2.43                     | 0.51              |
| 1:AA:1006:C:H2'    | 1:AA:1007:C:C5    | 2.46                     | 0.51              |
| 1:AA:1261:A:C2'    | 1:AA:1262:C:H5'   | 2.39                     | 0.51              |
| 1:AA:1270:C:H2'    | 1:AA:1271:G:H8    | 1.74                     | 0.51              |
| 1:AA:1430:C:C2     | 1:AA:1471:G:N2    | 2.79                     | 0.51              |
| 1:AA:296:U:O2'     | 1:AA:297:G:H5'    | 2.11                     | 0.51              |
| 1:AA:514:C:H2'     | 1:AA:515:G:H8     | 1.76                     | 0.51              |
| 1:AA:651:C:H2'     | 1:AA:652:U:C6     | 2.46                     | 0.51              |
| 1:AA:972:C:H4'     | 10:AJ:57:LYS:HB2  | 1.93                     | 0.51              |
| 3:AC:141:VAL:HG12  | 3:AC:146:ALA:HB3  | 1.92                     | 0.51              |
| 3:AC:207:VAL:HG12  | 3:AC:207:VAL:O    | 2.10                     | 0.51              |
| 6:AF:15:ASP:C      | 6:AF:17:SER:N     | 2.61                     | 0.51              |
| 16:AP:3:LYS:HG2    | 16:AP:65:GLN:HB2  | 1.92                     | 0.51              |
| 20:AT:57:ARG:HH11  | 20:AT:102:GLY:HA2 | 1.76                     | 0.51              |
| 24:AY:15:ILE:O     | 24:AY:15:ILE:HD12 | 2.11                     | 0.51              |
| 29:B4:1:MET:SD     | 41:BG:98:ARG:CG   | 2.99                     | 0.51              |
| 31:B6:9:LEU:O      | 31:B6:9:LEU:HD13  | 2.11                     | 0.51              |
| 33:B8:28:GLY:HA2   | 33:B8:32:LEU:HD21 | 1.92                     | 0.51              |
| 35:BA:20:C:H2'     | 35:BA:21:A:H8     | 1.76                     | 0.51              |
| 35:BA:2306:C:C5    | 35:BA:2307:G:O2'  | 2.63                     | 0.51              |
| 35:BA:2705:A:H2'   | 35:BA:2706:G:O4'  | 2.11                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:2870:C:O2'   | 35:BA:2871:C:H5'   | 2.11                     | 0.51              |
| 35:BA:650:C:C2'    | 35:BA:651:G:H5''   | 2.41                     | 0.51              |
| 36:BB:87:G:C2'     | 36:BB:88:C:H5''    | 2.40                     | 0.51              |
| 37:BC:60:ARG:HG2   | 37:BC:61:GLY:H     | 1.75                     | 0.51              |
| 38:BD:210:GLY:O    | 38:BD:211:ARG:HB3  | 2.11                     | 0.51              |
| 39:BE:111:ARG:CZ   | 50:BR:2:ARG:HH21   | 2.24                     | 0.51              |
| 35:BA:2810:A:H2'   | 39:BE:61:ARG:NH2   | 2.26                     | 0.51              |
| 39:BE:87:GLU:O     | 39:BE:89:ASP:N     | 2.44                     | 0.51              |
| 40:BF:127:GLU:HB2  | 40:BF:196:LEU:HD11 | 1.93                     | 0.51              |
| 42:BH:83:TYR:CB    | 42:BH:134:SER:HA   | 2.37                     | 0.51              |
| 42:BH:16:SER:HB2   | 42:BH:27:LYS:CB    | 2.35                     | 0.51              |
| 46:BN:102:ALA:O    | 46:BN:106:MET:CE   | 2.58                     | 0.51              |
| 46:BN:95:PRO:HA    | 46:BN:98:VAL:HG23  | 1.93                     | 0.51              |
| 49:BQ:2:LEU:HG     | 49:BQ:69:PHE:CE1   | 2.46                     | 0.51              |
| 50:BR:117:VAL:O    | 50:BR:118:GLU:CB   | 2.57                     | 0.51              |
| 35:BA:2820:A:O3'   | 50:BR:5:LYS:HE3    | 2.11                     | 0.51              |
| 54:BV:62:LEU:N     | 54:BV:62:LEU:HD22  | 2.26                     | 0.51              |
| 54:BV:93:GLU:O     | 54:BV:94:LEU:HD23  | 2.11                     | 0.51              |
| 56:BX:70:LEU:C     | 56:BX:70:LEU:HD23  | 2.31                     | 0.51              |
| 57:BY:10:GLY:O     | 57:BY:27:VAL:HG22  | 2.11                     | 0.51              |
| 58:BZ:40:ASP:HB3   | 58:BZ:43:GLU:HG2   | 1.92                     | 0.51              |
| 1:CA:1029:C:O2'    | 1:CA:1032:G:N2     | 2.44                     | 0.51              |
| 1:CA:1202:G:C2'    | 1:CA:1203:C:H5'    | 2.40                     | 0.51              |
| 1:CA:1366:C:H2'    | 1:CA:1367:C:C6     | 2.46                     | 0.51              |
| 1:CA:229:U:O2'     | 1:CA:230:G:H5'     | 2.10                     | 0.51              |
| 1:CA:353:A:H5'     | 1:CA:353:A:C8      | 2.41                     | 0.51              |
| 2:CB:95:GLN:HE21   | 2:CB:147:LYS:HE3   | 1.75                     | 0.51              |
| 3:CC:151:VAL:HG12  | 3:CC:152:ILE:N     | 2.25                     | 0.51              |
| 5:CE:77:PRO:HG2    | 5:CE:78:HIS:H      | 1.76                     | 0.51              |
| 6:CF:24:GLU:OE2    | 6:CF:28:ARG:NH1    | 2.44                     | 0.51              |
| 7:CG:5:ARG:HD2     | 7:CG:5:ARG:N       | 2.26                     | 0.51              |
| 1:CA:878:G:H5'     | 8:CH:89:PRO:HG2    | 1.92                     | 0.51              |
| 9:CI:5:TYR:O       | 9:CI:84:ALA:HA     | 2.10                     | 0.51              |
| 13:CM:116:THR:CG2  | 13:CM:117:VAL:N    | 2.74                     | 0.51              |
| 20:CT:13:LEU:O     | 20:CT:16:HIS:N     | 2.44                     | 0.51              |
| 24:CY:106:VAL:HG12 | 24:CY:108:PHE:CE1  | 2.46                     | 0.51              |
| 24:CY:191:ASP:O    | 24:CY:193:GLY:N    | 2.44                     | 0.51              |
| 24:CY:330:VAL:HG12 | 24:CY:331:TYR:N    | 2.25                     | 0.51              |
| 24:CY:631:ILE:HG23 | 24:CY:632:LEU:N    | 2.26                     | 0.51              |
| 27:D2:3:LEU:HD22   | 27:D2:7:ARG:NH2    | 2.25                     | 0.51              |
| 32:D7:48:LYS:HZ3   | 35:DA:125:G:H21    | 1.58                     | 0.51              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:1216:G:N2    | 35:DA:1234:U:H1'   | 2.26                     | 0.51              |
| 35:DA:2050:C:H2'   | 35:DA:2051:A:O4'   | 2.11                     | 0.51              |
| 35:DA:528:A:C2     | 35:DA:2043:C:C5'   | 2.94                     | 0.51              |
| 35:DA:753:C:H2'    | 35:DA:754:C:H6     | 1.75                     | 0.51              |
| 35:DA:768:G:H2'    | 35:DA:769:G:H8     | 1.76                     | 0.51              |
| 25:D0:77:ARG:NH2   | 35:DA:857:C:H5'    | 2.23                     | 0.51              |
| 36:DB:68:C:O2'     | 36:DB:69:G:H5'     | 2.11                     | 0.51              |
| 36:DB:81:G:H5'     | 36:DB:81:G:N3      | 2.26                     | 0.51              |
| 37:DC:101:ILE:N    | 37:DC:101:ILE:HD12 | 2.26                     | 0.51              |
| 38:DD:148:GLU:HB2  | 38:DD:151:LYS:CG   | 2.41                     | 0.51              |
| 38:DD:270:ILE:O    | 38:DD:270:ILE:HD12 | 2.11                     | 0.51              |
| 39:DE:145:LYS:O    | 39:DE:148:GLY:N    | 2.44                     | 0.51              |
| 41:DG:100:TRP:O    | 41:DG:104:GLU:HB2  | 2.10                     | 0.51              |
| 41:DG:109:VAL:C    | 41:DG:112:PRO:HD2  | 2.31                     | 0.51              |
| 41:DG:55:LYS:HG2   | 41:DG:58:GLN:NE2   | 2.24                     | 0.51              |
| 52:DT:106:SER:C    | 52:DT:107:ASP:OD1  | 2.49                     | 0.51              |
| 52:DT:36:GLU:HG2   | 52:DT:36:GLU:O     | 2.11                     | 0.51              |
| 52:DT:82:LEU:HD23  | 52:DT:85:LYS:HD2   | 1.93                     | 0.51              |
| 58:DZ:167:PRO:HG2  | 58:DZ:167:PRO:O    | 2.11                     | 0.51              |
| 49:DQ:56:ARG:NH2   | 58:DZ:180:VAL:HG21 | 2.17                     | 0.51              |
| 1:AA:1089:G:O2'    | 1:AA:1090:U:H5'    | 2.11                     | 0.51              |
| 1:AA:229:U:O2'     | 1:AA:230:G:H5'     | 2.11                     | 0.51              |
| 2:AB:223:ILE:HG23  | 2:AB:226:ARG:HD2   | 1.93                     | 0.51              |
| 6:AF:3:ARG:HH11    | 6:AF:3:ARG:HG3     | 1.76                     | 0.51              |
| 9:AI:40:LEU:C      | 9:AI:42:ARG:H      | 2.14                     | 0.51              |
| 12:AL:41:ARG:CG    | 12:AL:42:THR:N     | 2.71                     | 0.51              |
| 13:AM:65:LYS:C     | 13:AM:66:LEU:HD12  | 2.30                     | 0.51              |
| 24:AY:170:ARG:C    | 24:AY:171:GLU:HG2  | 2.30                     | 0.51              |
| 24:AY:510:VAL:HG12 | 24:AY:511:LYS:N    | 2.25                     | 0.51              |
| 31:B6:12:GLU:HB3   | 31:B6:23:THR:HG22  | 1.93                     | 0.51              |
| 33:B8:29:LYS:HD2   | 33:B8:44:LYS:CB    | 2.41                     | 0.51              |
| 35:BA:1063:G:O2'   | 35:BA:1064:C:H5'   | 2.11                     | 0.51              |
| 35:BA:1095:A:H2'   | 35:BA:1096:A:C8    | 2.46                     | 0.51              |
| 35:BA:1192:G:H2'   | 35:BA:1193:G:O4'   | 2.11                     | 0.51              |
| 35:BA:190:A:H2'    | 35:BA:191:A:C8     | 2.46                     | 0.51              |
| 35:BA:909:A:O2'    | 35:BA:910:A:H5'    | 2.10                     | 0.51              |
| 35:BA:917:A:H2'    | 35:BA:918:A:O4'    | 2.11                     | 0.51              |
| 29:B4:3:GLU:HG3    | 36:BB:43:C:P       | 2.51                     | 0.51              |
| 38:BD:238:GLY:O    | 38:BD:239:ARG:O    | 2.29                     | 0.51              |
| 39:BE:51:PHE:CD1   | 39:BE:52:LEU:N     | 2.79                     | 0.51              |
| 41:BG:102:PHE:O    | 41:BG:103:LEU:C    | 2.48                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:BN:58:ASP:O     | 46:BN:60:ILE:HG13  | 2.11                     | 0.51              |
| 50:BR:45:ARG:CG    | 50:BR:46:GLY:H     | 2.16                     | 0.51              |
| 56:BX:14:SER:H     | 56:BX:17:ALA:HB3   | 1.76                     | 0.51              |
| 56:BX:35:THR:HG22  | 56:BX:36:LYS:N     | 2.26                     | 0.51              |
| 35:BA:65:C:H5'     | 56:BX:71:GLY:HA3   | 1.93                     | 0.51              |
| 57:BY:99:CYS:O     | 57:BY:100:ALA:O    | 2.27                     | 0.51              |
| 57:BY:86:ARG:H     | 57:BY:88:LYS:NZ    | 2.08                     | 0.51              |
| 1:CA:1292:U:H2'    | 1:CA:1293:G:H8     | 1.75                     | 0.51              |
| 1:CA:1392:G:N2     | 1:CA:1502:A:C8     | 2.78                     | 0.51              |
| 1:CA:445:G:H2'     | 1:CA:446:G:C8      | 2.45                     | 0.51              |
| 1:CA:444:C:H42     | 1:CA:490:G:H1      | 1.58                     | 0.51              |
| 1:CA:707:C:H4'     | 11:CK:20:TYR:CD1   | 2.46                     | 0.51              |
| 7:CG:105:VAL:O     | 7:CG:108:ALA:HB3   | 2.11                     | 0.51              |
| 7:CG:69:VAL:HG21   | 7:CG:104:LEU:CD2   | 2.40                     | 0.51              |
| 7:CG:81:GLY:O      | 7:CG:83:ALA:N      | 2.40                     | 0.51              |
| 15:CO:65:ARG:NH1   | 15:CO:65:ARG:HG2   | 2.25                     | 0.51              |
| 19:CS:16:LEU:N     | 19:CS:16:LEU:HD12  | 2.26                     | 0.51              |
| 19:CS:27:GLU:O     | 19:CS:28:LYS:O     | 2.29                     | 0.51              |
| 20:CT:86:ARG:HH11  | 20:CT:86:ARG:HG3   | 1.76                     | 0.51              |
| 24:CY:201:ILE:H    | 24:CY:201:ILE:CD1  | 2.15                     | 0.51              |
| 24:CY:238:THR:O    | 24:CY:240:GLU:N    | 2.44                     | 0.51              |
| 24:CY:355:LEU:HD22 | 24:CY:355:LEU:N    | 2.25                     | 0.51              |
| 28:D3:31:LEU:HD22  | 28:D3:32:GLN:N     | 2.25                     | 0.51              |
| 35:DA:1019:U:H3    | 35:DA:1142(A):A:N6 | 2.09                     | 0.51              |
| 35:DA:1218:C:H2'   | 35:DA:1219:G:H8    | 1.76                     | 0.51              |
| 35:DA:1692:U:H2'   | 35:DA:1694:C:C4    | 2.46                     | 0.51              |
| 35:DA:1780:A:H5'   | 35:DA:1781:C:OP2   | 2.11                     | 0.51              |
| 35:DA:2307:G:N3    | 35:DA:2307:G:H3'   | 2.26                     | 0.51              |
| 35:DA:2348:U:H2'   | 35:DA:2349:G:H5'   | 1.92                     | 0.51              |
| 35:DA:2367:G:H2'   | 35:DA:2368:C:H6    | 1.76                     | 0.51              |
| 35:DA:2617:C:C2'   | 35:DA:2618:G:H5'   | 2.41                     | 0.51              |
| 35:DA:363(A):A:H2' | 35:DA:363(B):G:C8  | 2.45                     | 0.51              |
| 35:DA:503:A:H4'    | 35:DA:504:U:H5'    | 1.93                     | 0.51              |
| 37:DC:135:ARG:HD2  | 37:DC:135:ARG:N    | 2.25                     | 0.51              |
| 37:DC:149:ASN:N    | 37:DC:149:ASN:HD22 | 2.08                     | 0.51              |
| 38:DD:166:GLN:NE2  | 38:DD:166:GLN:HA   | 2.26                     | 0.51              |
| 39:DE:63:LEU:O     | 39:DE:64:LYS:C     | 2.49                     | 0.51              |
| 40:DF:192:LEU:HD23 | 40:DF:193:VAL:N    | 2.25                     | 0.51              |
| 41:DG:123:ASN:C    | 41:DG:125:PHE:N    | 2.64                     | 0.51              |
| 41:DG:107:LEU:HD22 | 41:DG:177:GLY:O    | 2.10                     | 0.51              |
| 44:DK:120:LEU:HA   | 44:DK:123:ALA:HB3  | 1.93                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:DN:65:LYS:NZ    | 46:DN:65:LYS:HA    | 2.25                     | 0.51              |
| 35:DA:2470:G:P     | 49:DQ:56:ARG:NH1   | 2.83                     | 0.51              |
| 53:DU:33:ARG:C     | 53:DU:35:ALA:N     | 2.59                     | 0.51              |
| 46:DN:2:LYS:NZ     | 54:DV:12:TYR:HA    | 2.25                     | 0.51              |
| 54:DV:21:ARG:HB3   | 54:DV:91:TYR:HD1   | 1.71                     | 0.51              |
| 54:DV:49:THR:O     | 54:DV:50:PRO:C     | 2.47                     | 0.51              |
| 57:DY:95:LYS:HE2   | 57:DY:101:LYS:H    | 1.76                     | 0.51              |
| 1:AA:1298:C:C2'    | 1:AA:1298:C:O2     | 2.60                     | 0.50              |
| 1:AA:1333:A:C2     | 1:AA:1334:G:H1'    | 2.46                     | 0.50              |
| 1:AA:1493:A:H8     | 1:AA:1493:A:OP2    | 1.93                     | 0.50              |
| 3:AC:155:GLY:O     | 3:AC:156:ARG:HB2   | 2.10                     | 0.50              |
| 4:AD:155:LEU:O     | 4:AD:156:GLU:C     | 2.49                     | 0.50              |
| 5:AE:139:LEU:C     | 5:AE:141:GLN:H     | 2.14                     | 0.50              |
| 24:AY:236:GLU:HG3  | 24:AY:236:GLU:O    | 2.10                     | 0.50              |
| 24:AY:177:ILE:HG21 | 24:AY:260:LEU:HD21 | 1.93                     | 0.50              |
| 24:AY:635:GLU:OE1  | 24:AY:644:ARG:HD2  | 2.11                     | 0.50              |
| 26:B1:92:LYS:HE2   | 35:BA:153:C:OP1    | 2.11                     | 0.50              |
| 27:B2:15:LYS:O     | 27:B2:15:LYS:HG3   | 2.10                     | 0.50              |
| 27:B2:8:LYS:O      | 27:B2:12:GLU:N     | 2.29                     | 0.50              |
| 28:B3:54:VAL:HG12  | 28:B3:55:ARG:N     | 2.26                     | 0.50              |
| 35:BA:1216:G:N2    | 35:BA:1234:U:H1'   | 2.26                     | 0.50              |
| 35:BA:1378:A:HO2'  | 35:BA:1379:A:H5''  | 1.69                     | 0.50              |
| 35:BA:1784:A:H4'   | 35:BA:1785:A:O5'   | 2.11                     | 0.50              |
| 35:BA:1917:U:H2'   | 35:BA:1918:A:H5'   | 1.93                     | 0.50              |
| 35:BA:654(M):C:O2' | 35:BA:654(N):G:C8  | 2.58                     | 0.50              |
| 35:BA:750:A:C2     | 35:BA:753:C:C6     | 2.99                     | 0.50              |
| 39:BE:4:ILE:HG13   | 39:BE:5:LEU:H      | 1.75                     | 0.50              |
| 39:BE:59:VAL:HG21  | 39:BE:63:LEU:HA    | 1.92                     | 0.50              |
| 39:BE:81:ILE:O     | 39:BE:81:ILE:CG2   | 2.58                     | 0.50              |
| 41:BG:133:LEU:HD11 | 41:BG:157:ILE:CD1  | 2.29                     | 0.50              |
| 41:BG:46:ALA:HA    | 41:BG:51:ARG:CB    | 2.41                     | 0.50              |
| 46:BN:49:GLY:CA    | 46:BN:119:ARG:HH12 | 2.23                     | 0.50              |
| 46:BN:78:TYR:N     | 46:BN:78:TYR:CD1   | 2.79                     | 0.50              |
| 49:BQ:35:VAL:HG22  | 49:BQ:36:ALA:N     | 2.26                     | 0.50              |
| 49:BQ:75:THR:CG2   | 49:BQ:76:LYS:N     | 2.74                     | 0.50              |
| 50:BR:12:ARG:CG    | 50:BR:12:ARG:HH11  | 2.23                     | 0.50              |
| 53:BU:39:LEU:O     | 53:BU:40:PHE:C     | 2.48                     | 0.50              |
| 53:BU:8:VAL:CG2    | 53:BU:12:ARG:HE    | 2.24                     | 0.50              |
| 54:BV:79:VAL:O     | 54:BV:80:GLN:HB2   | 2.09                     | 0.50              |
| 56:BX:44:GLU:HB2   | 56:BX:49:VAL:O     | 2.11                     | 0.50              |
| 57:BY:43:ASN:HA    | 57:BY:64:GLU:HA    | 1.93                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 58:BZ:129:SER:C   | 58:BZ:131:ARG:H    | 2.14                     | 0.50              |
| 1:CA:22:G:H4'     | 1:CA:885:G:C8      | 2.46                     | 0.50              |
| 1:CA:893:C:H2'    | 1:CA:894:G:H8      | 1.76                     | 0.50              |
| 2:CB:121:LEU:HD21 | 2:CB:126:GLU:OE2   | 2.11                     | 0.50              |
| 2:CB:19:HIS:HD2   | 2:CB:189:ASP:OD2   | 1.94                     | 0.50              |
| 4:CD:120:LEU:HB3  | 4:CD:126:ILE:HD11  | 1.93                     | 0.50              |
| 5:CE:101:ILE:HG12 | 5:CE:101:ILE:O     | 2.10                     | 0.50              |
| 5:CE:59:GLY:O     | 5:CE:62:ALA:HB3    | 2.11                     | 0.50              |
| 10:CJ:4:ILE:H     | 10:CJ:4:ILE:HD12   | 1.77                     | 0.50              |
| 10:CJ:61:GLU:HG3  | 14:CN:58:LYS:CE    | 2.41                     | 0.50              |
| 15:CO:31:LEU:CD2  | 15:CO:31:LEU:H     | 2.23                     | 0.50              |
| 16:CP:19:ILE:N    | 16:CP:37:GLY:O     | 2.41                     | 0.50              |
| 18:CR:69:THR:O    | 18:CR:72:ARG:N     | 2.43                     | 0.50              |
| 19:CS:24:ALA:O    | 19:CS:25:LYS:CB    | 2.59                     | 0.50              |
| 24:CY:211:GLU:HB2 | 24:CY:215:LYS:HZ1  | 1.76                     | 0.50              |
| 24:CY:36:THR:OG1  | 24:CY:37:GLY:N     | 2.44                     | 0.50              |
| 24:CY:77:HIS:NE2  | 24:CY:277:VAL:HG21 | 2.27                     | 0.50              |
| 27:D2:67:LYS:O    | 27:D2:70:GLN:HG3   | 2.11                     | 0.50              |
| 31:D6:15:GLU:OE1  | 31:D6:41:PRO:CG    | 2.59                     | 0.50              |
| 33:D8:10:ALA:O    | 33:D8:14:VAL:HG12  | 2.10                     | 0.50              |
| 33:D8:39:LYS:HG3  | 33:D8:43:GLN:NE2   | 2.26                     | 0.50              |
| 35:DA:1708:C:O2'  | 35:DA:1709:U:H5'   | 2.11                     | 0.50              |
| 35:DA:2346:A:H1'  | 35:DA:2383:G:N9    | 2.25                     | 0.50              |
| 35:DA:2647:U:H2'  | 35:DA:2648:C:H6    | 1.74                     | 0.50              |
| 35:DA:2787:C:C2   | 39:DE:61:ARG:HD3   | 2.46                     | 0.50              |
| 26:D1:69:LYS:NZ   | 35:DA:372:G:OP2    | 2.42                     | 0.50              |
| 35:DA:558:G:H5'   | 46:DN:112:LEU:HD22 | 1.91                     | 0.50              |
| 35:DA:657:U:H2'   | 35:DA:658:C:H6     | 1.73                     | 0.50              |
| 37:DC:29:LEU:O    | 37:DC:31:LYS:N     | 2.44                     | 0.50              |
| 37:DC:60:ARG:HG2  | 37:DC:61:GLY:H     | 1.75                     | 0.50              |
| 41:DG:116:ASP:O   | 41:DG:117:PHE:CB   | 2.56                     | 0.50              |
| 41:DG:131:TYR:HB3 | 41:DG:159:VAL:CG1  | 2.41                     | 0.50              |
| 42:DH:33:LEU:HD12 | 42:DH:75:ALA:O     | 2.11                     | 0.50              |
| 42:DH:40:GLU:HG3  | 42:DH:64:LEU:CD1   | 2.41                     | 0.50              |
| 48:DP:128:HIS:ND1 | 48:DP:148:LEU:HD13 | 2.25                     | 0.50              |
| 48:DP:55:ARG:CG   | 48:DP:56:SER:N     | 2.64                     | 0.50              |
| 48:DP:67:MET:O    | 48:DP:68:GLN:HG3   | 2.10                     | 0.50              |
| 49:DQ:60:ARG:HB2  | 49:DQ:60:ARG:CZ    | 2.41                     | 0.50              |
| 52:DT:99:LEU:HB2  | 52:DT:101:PHE:HE1  | 1.76                     | 0.50              |
| 54:DV:66:ARG:NH1  | 54:DV:88:ARG:HE    | 2.09                     | 0.50              |
| 58:DZ:109:ALA:HB3 | 58:DZ:145:GLU:CA   | 2.42                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:DZ:151:HIS:HA   | 58:DZ:171:ILE:CG2  | 2.33                     | 0.50              |
| 1:AA:999:C:H2'     | 1:AA:1000:U:C4     | 2.45                     | 0.50              |
| 1:AA:1161:C:O2'    | 1:AA:1162:C:H5'    | 2.11                     | 0.50              |
| 1:AA:1190:G:OP1    | 3:AC:4:LYS:HA      | 2.11                     | 0.50              |
| 1:AA:260:G:H2'     | 1:AA:261:U:H6      | 1.75                     | 0.50              |
| 1:AA:542:G:O2'     | 1:AA:543:C:H5'     | 2.10                     | 0.50              |
| 1:AA:1112:C:O2'    | 3:AC:179:ARG:HG2   | 2.11                     | 0.50              |
| 3:AC:61:ALA:O      | 3:AC:62:ASP:HB2    | 2.10                     | 0.50              |
| 5:AE:77:PRO:HG2    | 5:AE:78:HIS:H      | 1.75                     | 0.50              |
| 10:AJ:4:ILE:CD1    | 10:AJ:74:ILE:HG13  | 2.40                     | 0.50              |
| 13:AM:66:LEU:O     | 13:AM:70:LEU:HB3   | 2.11                     | 0.50              |
| 24:AY:181:LEU:HB2  | 24:AY:216:LEU:HD11 | 1.93                     | 0.50              |
| 24:AY:407:PRO:HB3  | 24:AY:452:SER:OG   | 2.11                     | 0.50              |
| 24:AY:64:THR:C     | 24:AY:66:THR:H     | 2.14                     | 0.50              |
| 26:B1:76:ARG:HH22  | 26:B1:95:LEU:CD1   | 2.24                     | 0.50              |
| 30:B5:16:ARG:NH1   | 30:B5:17:ASP:OD1   | 2.44                     | 0.50              |
| 30:B5:2:ALA:O      | 30:B5:3:LYS:HB3    | 2.11                     | 0.50              |
| 31:B6:17:LYS:O     | 31:B6:20:ASN:ND2   | 2.44                     | 0.50              |
| 33:B8:48:PHE:O     | 33:B8:49:VAL:CG1   | 2.58                     | 0.50              |
| 35:BA:1204:A:H61   | 35:BA:1240:U:H2'   | 1.76                     | 0.50              |
| 35:BA:2121:G:O2'   | 37:BC:168:LYS:HG2  | 2.10                     | 0.50              |
| 35:BA:2298:A:N6    | 35:BA:2318:G:H8    | 2.09                     | 0.50              |
| 35:BA:2337:G:H2'   | 35:BA:2338:G:H8    | 1.75                     | 0.50              |
| 35:BA:2577:A:H5'   | 35:BA:2578:G:C5'   | 2.41                     | 0.50              |
| 35:BA:2688:U:H3'   | 35:BA:2688:U:O2    | 2.11                     | 0.50              |
| 35:BA:2735:G:H2'   | 35:BA:2736:G:C8    | 2.44                     | 0.50              |
| 35:BA:482:A:H4'    | 57:BY:47:LYS:HG2   | 1.93                     | 0.50              |
| 35:BA:651:G:C2'    | 35:BA:652:C:H5'    | 2.41                     | 0.50              |
| 35:BA:768:G:H2'    | 35:BA:769:G:C8     | 2.47                     | 0.50              |
| 25:B0:74:ARG:HG2   | 36:BB:13:A:OP2     | 2.12                     | 0.50              |
| 36:BB:81:G:N3      | 36:BB:81:G:H5'     | 2.26                     | 0.50              |
| 37:BC:101:ILE:HD12 | 37:BC:101:ILE:N    | 2.26                     | 0.50              |
| 41:BG:152:LEU:CD2  | 41:BG:152:LEU:H    | 2.23                     | 0.50              |
| 44:BK:136:VAL:HG13 | 44:BK:136:VAL:O    | 2.11                     | 0.50              |
| 44:BK:78:ILE:HD13  | 44:BK:134:MET:SD   | 2.51                     | 0.50              |
| 47:BO:105:GLU:O    | 47:BO:109:LYS:CG   | 2.57                     | 0.50              |
| 35:BA:2870:C:H5''  | 50:BR:65:LEU:HD21  | 1.92                     | 0.50              |
| 51:BS:85:VAL:HG23  | 51:BS:106:ARG:CG   | 2.41                     | 0.50              |
| 51:BS:25:ARG:HG3   | 51:BS:26:LEU:H     | 1.77                     | 0.50              |
| 53:BU:95:LEU:CD1   | 54:BV:11:GLN:HG3   | 2.41                     | 0.50              |
| 54:BV:19:LYS:HB3   | 54:BV:94:LEU:O     | 2.11                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1220:G:H2'    | 1:CA:1221:G:C8     | 2.46                     | 0.50              |
| 1:CA:1268:A:H2'    | 1:CA:1269:A:C8     | 2.46                     | 0.50              |
| 1:CA:1287:A:H2'    | 1:CA:1288:A:C8     | 2.46                     | 0.50              |
| 1:CA:892:A:O2'     | 1:CA:1415:G:H4'    | 2.11                     | 0.50              |
| 1:CA:418:C:H2'     | 1:CA:419:C:C6      | 2.46                     | 0.50              |
| 1:CA:821:G:O2'     | 1:CA:822:C:H5'     | 2.11                     | 0.50              |
| 2:CB:91:PRO:HG2    | 2:CB:155:LEU:HD23  | 1.92                     | 0.50              |
| 3:CC:173:VAL:HG12  | 3:CC:175:LEU:CD1   | 2.41                     | 0.50              |
| 3:CC:10:PHE:CE1    | 3:CC:178:LEU:HD11  | 2.46                     | 0.50              |
| 4:CD:58:LEU:O      | 4:CD:58:LEU:HD23   | 2.11                     | 0.50              |
| 4:CD:61:LYS:NZ     | 4:CD:72:GLU:OE2    | 2.40                     | 0.50              |
| 5:CE:41:VAL:HG13   | 5:CE:113:ALA:HA    | 1.91                     | 0.50              |
| 5:CE:101:ILE:CD1   | 5:CE:119:LEU:HA    | 2.29                     | 0.50              |
| 7:CG:78:ARG:HE     | 7:CG:156:TRP:HB3   | 1.75                     | 0.50              |
| 8:CH:41:ARG:NH2    | 8:CH:123:GLU:CD    | 2.64                     | 0.50              |
| 1:CA:190:U:C2      | 20:CT:105:SER:HB2  | 2.46                     | 0.50              |
| 24:CY:191:ASP:C    | 24:CY:193:GLY:N    | 2.65                     | 0.50              |
| 24:CY:369:LEU:N    | 24:CY:369:LEU:HD12 | 2.25                     | 0.50              |
| 24:CY:606:MET:HE3  | 24:CY:671:MET:CG   | 2.41                     | 0.50              |
| 26:D1:90:ILE:HG22  | 26:D1:94:LEU:HD11  | 1.92                     | 0.50              |
| 27:D2:3:LEU:HD12   | 35:DA:98:G:C5'     | 2.41                     | 0.50              |
| 35:DA:1040:C:H2'   | 35:DA:1041:C:C6    | 2.46                     | 0.50              |
| 35:DA:1542:A:H3'   | 35:DA:1542:A:H8    | 1.75                     | 0.50              |
| 35:DA:1891:G:H2'   | 35:DA:1892:C:O4'   | 2.11                     | 0.50              |
| 35:DA:2723:C:H5''  | 50:DR:2:ARG:NH1    | 2.15                     | 0.50              |
| 35:DA:2860:A:H2'   | 35:DA:2861:G:H5'   | 1.93                     | 0.50              |
| 35:DA:567:A:N1     | 35:DA:571:A:H8     | 2.08                     | 0.50              |
| 35:DA:658:C:H2'    | 35:DA:659:C:C6     | 2.47                     | 0.50              |
| 35:DA:705:A:C2     | 35:DA:727:A:H1'    | 2.46                     | 0.50              |
| 42:DH:105:LEU:N    | 42:DH:105:LEU:HD23 | 2.27                     | 0.50              |
| 44:DK:136:VAL:HG13 | 44:DK:136:VAL:O    | 2.11                     | 0.50              |
| 49:DQ:79:LEU:HD23  | 49:DQ:80:GLU:N     | 2.24                     | 0.50              |
| 50:DR:7:GLY:C      | 50:DR:8:ARG:HE     | 2.14                     | 0.50              |
| 51:DS:101:LEU:HD12 | 51:DS:101:LEU:C    | 2.30                     | 0.50              |
| 53:DU:83:LEU:HD12  | 53:DU:113:ALA:HB2  | 1.92                     | 0.50              |
| 53:DU:92:ARG:HD3   | 53:DU:94:ASN:CB    | 2.41                     | 0.50              |
| 58:DZ:64:GLY:O     | 58:DZ:65:GLN:C     | 2.49                     | 0.50              |
| 1:AA:1505:G:H4'    | 1:AA:1506:U:H5''   | 1.93                     | 0.50              |
| 1:AA:190:U:C2      | 20:AT:105:SER:HB2  | 2.46                     | 0.50              |
| 1:AA:445:G:H2'     | 1:AA:446:G:C8      | 2.46                     | 0.50              |
| 1:AA:980:C:H2'     | 1:AA:981:U:H5'     | 1.93                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 2:AB:233:SER:OG   | 2:AB:234:PRO:HD2    | 2.11                     | 0.50              |
| 9:AI:79:LEU:O     | 9:AI:80:GLY:C       | 2.49                     | 0.50              |
| 13:AM:56:LEU:HD13 | 13:AM:56:LEU:C      | 2.31                     | 0.50              |
| 19:AS:19:VAL:HG12 | 19:AS:20:LEU:HG     | 1.94                     | 0.50              |
| 24:AY:114:VAL:O   | 24:AY:116:PRO:HD3   | 2.11                     | 0.50              |
| 24:AY:252:ASP:HB2 | 24:AY:254:LYS:CG    | 2.40                     | 0.50              |
| 24:AY:35:TYR:CE1  | 24:AY:269:VAL:HB    | 2.45                     | 0.50              |
| 24:AY:415:PRO:CB  | 24:AY:421:GLN:HA    | 2.42                     | 0.50              |
| 24:AY:485:GLU:OE1 | 24:AY:555:LEU:HB2   | 2.12                     | 0.50              |
| 24:AY:634:MET:O   | 24:AY:634:MET:HG2   | 2.10                     | 0.50              |
| 24:AY:71:THR:HG21 | 24:AY:357:ARG:CD    | 2.41                     | 0.50              |
| 31:B6:47:THR:CG2  | 31:B6:48:VAL:H      | 2.19                     | 0.50              |
| 35:BA:1542:A:C8   | 35:BA:1542:A:H3'    | 2.46                     | 0.50              |
| 35:BA:1610:A:H4'  | 35:BA:1611:C:OP2    | 2.11                     | 0.50              |
| 35:BA:1680:U:O2'  | 35:BA:1681:G:H5'    | 2.12                     | 0.50              |
| 35:BA:1814:G:H4'  | 38:BD:51:VAL:HG21   | 1.92                     | 0.50              |
| 35:BA:2130:U:OP1  | 37:BC:6:LYS:HB2     | 2.11                     | 0.50              |
| 35:BA:2192:G:C3'  | 35:BA:2193:G:H5''   | 2.42                     | 0.50              |
| 35:BA:2307:G:N2   | 35:BA:2308:G:C5'    | 2.74                     | 0.50              |
| 35:BA:2712:U:C2'  | 35:BA:2712(A):A:O5' | 2.60                     | 0.50              |
| 35:BA:2867:G:N7   | 52:BT:23:ARG:NH1    | 2.58                     | 0.50              |
| 35:BA:588:U:H1'   | 40:BF:90:PHE:CG     | 2.47                     | 0.50              |
| 35:BA:958:U:H3'   | 35:BA:958:U:C6      | 2.46                     | 0.50              |
| 37:BC:92:ALA:HB3  | 37:BC:95:VAL:HG22   | 1.92                     | 0.50              |
| 38:BD:108:PRO:HG2 | 38:BD:111:LEU:HB2   | 1.92                     | 0.50              |
| 38:BD:145:VAL:CG1 | 38:BD:146:GLU:N     | 2.75                     | 0.50              |
| 38:BD:62:TYR:CE1  | 38:BD:64:ILE:HA     | 2.45                     | 0.50              |
| 39:BE:32:PRO:N    | 39:BE:90:THR:HG23   | 2.27                     | 0.50              |
| 39:BE:61:ARG:HG2  | 39:BE:62:PRO:CD     | 2.41                     | 0.50              |
| 40:BF:192:LEU:CD2 | 40:BF:194:MET:HG3   | 2.30                     | 0.50              |
| 42:BH:54:ARG:HD2  | 42:BH:54:ARG:O      | 2.11                     | 0.50              |
| 45:BL:14:UNK:HA   | 45:BM:13:UNK:O      | 26.78                    | 0.50              |
| 47:BO:107:ARG:HA  | 47:BO:112:MET:CE    | 2.41                     | 0.50              |
| 48:BP:58:THR:O    | 48:BP:58:THR:HG22   | 2.11                     | 0.50              |
| 49:BQ:135:ASP:O   | 49:BQ:138:ASP:OD2   | 2.30                     | 0.50              |
| 51:BS:73:LEU:O    | 51:BS:73:LEU:HD23   | 2.12                     | 0.50              |
| 53:BU:79:PHE:O    | 53:BU:83:LEU:HD13   | 2.11                     | 0.50              |
| 58:BZ:45:ASP:OD2  | 58:BZ:49:ARG:HG2    | 2.11                     | 0.50              |
| 1:CA:1006:C:H2'   | 1:CA:1007:C:C5      | 2.47                     | 0.50              |
| 1:CA:1507:A:C2    | 1:CA:1508:G:C4      | 2.99                     | 0.50              |
| 1:CA:193:C:H2'    | 1:CA:194:C:C6       | 2.47                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:260:G:H2'     | 1:CA:261:U:C6      | 2.46                     | 0.50              |
| 1:CA:264:U:O2'     | 17:CQ:64:PRO:HB2   | 2.11                     | 0.50              |
| 1:CA:664:G:O2'     | 1:CA:666:G:OP2     | 2.28                     | 0.50              |
| 1:CA:779:C:O2'     | 11:CK:120:ARG:HD3  | 2.10                     | 0.50              |
| 2:CB:172:ILE:CD1   | 2:CB:172:ILE:H     | 2.04                     | 0.50              |
| 4:CD:153:ARG:HG2   | 4:CD:153:ARG:NH1   | 2.26                     | 0.50              |
| 10:CJ:58:ASP:O     | 10:CJ:59:SER:C     | 2.50                     | 0.50              |
| 10:CJ:63:PHE:HA    | 14:CN:59:ALA:CB    | 2.40                     | 0.50              |
| 12:CL:27:LEU:C     | 12:CL:29:GLY:N     | 2.64                     | 0.50              |
| 12:CL:38:THR:HG23  | 12:CL:57:LYS:CB    | 2.42                     | 0.50              |
| 12:CL:6:THR:HG23   | 12:CL:9:GLN:NE2    | 2.24                     | 0.50              |
| 12:CL:97:ARG:C     | 12:CL:98:TYR:CD1   | 2.84                     | 0.50              |
| 15:CO:17:ARG:NH1   | 15:CO:77:ARG:CZ    | 2.74                     | 0.50              |
| 24:CY:526:VAL:HG11 | 24:CY:566:THR:HG23 | 1.94                     | 0.50              |
| 24:CY:82:ILE:HD12  | 24:CY:101:LEU:CD2  | 2.41                     | 0.50              |
| 27:D2:48:HIS:CG    | 27:D2:49:LYS:H     | 2.29                     | 0.50              |
| 29:D4:14:ILE:HG22  | 29:D4:15:ILE:N     | 2.25                     | 0.50              |
| 31:D6:9:LEU:HD22   | 31:D6:9:LEU:C      | 2.32                     | 0.50              |
| 35:DA:1145:C:H2'   | 35:DA:1146:C:C6    | 2.46                     | 0.50              |
| 35:DA:1858:G:HO2'  | 35:DA:1859:A:H8    | 1.59                     | 0.50              |
| 35:DA:2053:G:H1    | 35:DA:2616:C:H42   | 1.59                     | 0.50              |
| 35:DA:2306:C:C5    | 35:DA:2307:G:O2'   | 2.61                     | 0.50              |
| 30:D5:22:HIS:CE1   | 35:DA:2624:G:H1'   | 2.46                     | 0.50              |
| 35:DA:2678:C:O2'   | 35:DA:2679:A:H5'   | 2.11                     | 0.50              |
| 35:DA:2816:C:O2    | 35:DA:2883:A:O2'   | 2.30                     | 0.50              |
| 35:DA:572:A:OP2    | 54:DV:78:LYS:NZ    | 2.38                     | 0.50              |
| 35:DA:665:C:H2'    | 35:DA:666:G:H8     | 1.76                     | 0.50              |
| 36:DB:87:G:C2'     | 36:DB:88:C:H5''    | 2.41                     | 0.50              |
| 35:DA:1567:A:C5'   | 38:DD:58:HIS:CD2   | 2.94                     | 0.50              |
| 39:DE:101:ARG:NH1  | 39:DE:169:ASN:ND2  | 2.59                     | 0.50              |
| 39:DE:24:THR:CG2   | 39:DE:184:VAL:HG23 | 2.39                     | 0.50              |
| 40:DF:123:LEU:HD12 | 40:DF:124:LEU:H    | 1.74                     | 0.50              |
| 42:DH:172:LYS:HG3  | 42:DH:175:LYS:CE   | 2.42                     | 0.50              |
| 46:DN:89:LYS:O     | 46:DN:93:THR:HG22  | 2.12                     | 0.50              |
| 47:DO:10:VAL:HG23  | 47:DO:10:VAL:O     | 2.11                     | 0.50              |
| 35:DA:624:C:H41    | 48:DP:107:LYS:HZ2  | 1.59                     | 0.50              |
| 48:DP:121:LYS:O    | 48:DP:123:LEU:HD23 | 2.11                     | 0.50              |
| 51:DS:93:LYS:O     | 51:DS:94:TYR:C     | 2.49                     | 0.50              |
| 52:DT:12:SER:O     | 52:DT:13:ARG:NH2   | 2.44                     | 0.50              |
| 1:AA:1002:G:N2     | 1:AA:1039:C:H2'    | 2.25                     | 0.50              |
| 1:AA:691:G:H2'     | 1:AA:692:U:C6      | 2.46                     | 0.50              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:708:C:H2'     | 1:AA:709:G:H8      | 1.77                     | 0.50              |
| 1:AA:707:C:O2'     | 1:AA:708:C:H5'     | 2.11                     | 0.50              |
| 7:AG:78:ARG:HG3    | 7:AG:78:ARG:HH11   | 1.76                     | 0.50              |
| 8:AH:9:MET:O       | 8:AH:13:ILE:HG12   | 2.11                     | 0.50              |
| 11:AK:17:GLY:O     | 11:AK:80:VAL:HA    | 2.12                     | 0.50              |
| 12:AL:80:HIS:O     | 12:AL:81:SER:CB    | 2.58                     | 0.50              |
| 1:AA:1202:G:C2     | 14:AN:42:ILE:HG21  | 2.47                     | 0.50              |
| 18:AR:56:THR:CB    | 18:AR:58:LEU:HD13  | 2.37                     | 0.50              |
| 22:AW:53:G:H2'     | 22:AW:54:G:C8      | 2.47                     | 0.50              |
| 24:AY:214:GLU:O    | 24:AY:218:GLU:N    | 2.42                     | 0.50              |
| 24:AY:293:THR:HA   | 24:AY:397:VAL:HG12 | 1.94                     | 0.50              |
| 24:AY:428:LEU:N    | 24:AY:428:LEU:HD23 | 2.25                     | 0.50              |
| 24:AY:427:ALA:O    | 24:AY:431:LEU:HB2  | 2.12                     | 0.50              |
| 25:B0:40:GLN:HE22  | 25:B0:43:THR:CA    | 2.22                     | 0.50              |
| 26:B1:64:ALA:HA    | 26:B1:67:ILE:CG1   | 2.41                     | 0.50              |
| 26:B1:80:LEU:HD13  | 26:B1:82:LEU:HD11  | 1.94                     | 0.50              |
| 35:BA:1493:C:O2    | 35:BA:1493:C:H2'   | 2.10                     | 0.50              |
| 35:BA:154(A):C:C5  | 35:BA:155:U:H1'    | 2.47                     | 0.50              |
| 35:BA:1567:A:H5'   | 38:BD:58:HIS:CD2   | 2.46                     | 0.50              |
| 35:BA:2392:A:H2    | 35:BA:2424:C:H42   | 1.60                     | 0.50              |
| 35:BA:2626:C:H2'   | 35:BA:2627:G:O4'   | 2.11                     | 0.50              |
| 35:BA:2736:G:O2'   | 35:BA:2737:G:H5'   | 2.12                     | 0.50              |
| 35:BA:2853:C:H2'   | 35:BA:2854:G:H8    | 1.77                     | 0.50              |
| 35:BA:381:G:O2'    | 35:BA:382:G:H5'    | 2.12                     | 0.50              |
| 35:BA:568:U:H2'    | 35:BA:570:G:OP2    | 2.11                     | 0.50              |
| 31:B6:42:TRP:NE1   | 35:BA:643:A:OP1    | 2.44                     | 0.50              |
| 37:BC:104:ILE:HG23 | 37:BC:108:TRP:O    | 2.11                     | 0.50              |
| 38:BD:142:VAL:HG23 | 38:BD:193:VAL:HA   | 1.93                     | 0.50              |
| 38:BD:43:ARG:CB    | 38:BD:54:ARG:HB2   | 2.41                     | 0.50              |
| 38:BD:35:LYS:CG    | 38:BD:63:ARG:HA    | 2.34                     | 0.50              |
| 42:BH:77:LYS:HA    | 42:BH:80:SER:OG    | 2.10                     | 0.50              |
| 35:BA:1058:G:H21   | 44:BK:126:MET:CE   | 2.24                     | 0.50              |
| 35:BA:624:C:N4     | 48:BP:107:LYS:NZ   | 2.60                     | 0.50              |
| 51:BS:93:LYS:O     | 51:BS:94:TYR:C     | 2.49                     | 0.50              |
| 52:BT:36:GLU:HG2   | 52:BT:36:GLU:O     | 2.11                     | 0.50              |
| 54:BV:66:ARG:NH1   | 54:BV:88:ARG:HE    | 2.10                     | 0.50              |
| 55:BW:66:GLU:HA    | 55:BW:69:LEU:CD1   | 2.41                     | 0.50              |
| 58:BZ:58:VAL:HA    | 58:BZ:67:LEU:O     | 2.12                     | 0.50              |
| 1:CA:999:C:H2'     | 1:CA:1000:U:C4     | 2.47                     | 0.50              |
| 1:CA:1089:G:O2'    | 1:CA:1090:U:H5'    | 2.11                     | 0.50              |
| 1:CA:1190:G:OP1    | 3:CC:4:LYS:HA      | 2.11                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1226:C:H5"    | 13:CM:103:THR:OG1  | 2.11                     | 0.50              |
| 1:CA:1525:G:O2'    | 1:CA:1526:G:H5'    | 2.12                     | 0.50              |
| 1:CA:187:C:OP1     | 20:CT:82:SER:HB2   | 2.10                     | 0.50              |
| 4:CD:119:GLN:HG3   | 4:CD:123:HIS:CD2   | 2.46                     | 0.50              |
| 5:CE:29:GLY:HA2    | 5:CE:46:GLY:O      | 2.11                     | 0.50              |
| 6:CF:38:GLU:HB2    | 6:CF:64:GLN:O      | 2.11                     | 0.50              |
| 8:CH:34:GLU:HB3    | 8:CH:118:VAL:HG21  | 1.92                     | 0.50              |
| 24:CY:142:THR:CG2  | 24:CY:143:GLY:N    | 2.75                     | 0.50              |
| 24:CY:165:GLN:NE2  | 24:CY:177:ILE:HG21 | 2.25                     | 0.50              |
| 24:CY:227:ILE:CD1  | 24:CY:242:LEU:HA   | 2.41                     | 0.50              |
| 24:CY:399:LEU:CD1  | 24:CY:399:LEU:N    | 2.74                     | 0.50              |
| 24:CY:413:ILE:HG23 | 24:CY:413:ILE:O    | 2.10                     | 0.50              |
| 24:CY:492:ASP:OD1  | 24:CY:513:LYS:HD2  | 2.12                     | 0.50              |
| 61:CY:702:FUA:O1   | 61:CY:702:FUA:C1   | 2.57                     | 0.50              |
| 25:D0:19:LYS:HD3   | 25:D0:41:ARG:NH2   | 2.26                     | 0.50              |
| 25:D0:27:GLU:HG3   | 25:D0:68:GLU:HA    | 1.93                     | 0.50              |
| 26:D1:84:GLY:O     | 26:D1:85:LEU:C     | 2.49                     | 0.50              |
| 35:DA:1367:A:C2'   | 35:DA:1368:G:H5'   | 2.40                     | 0.50              |
| 35:DA:1465:G:H2'   | 35:DA:1466:G:H8    | 1.75                     | 0.50              |
| 35:DA:154(A):C:H3' | 35:DA:155:U:H5"    | 1.93                     | 0.50              |
| 35:DA:443:A:H3'    | 40:DF:45:ARG:NH2   | 2.26                     | 0.50              |
| 35:DA:825:C:H2'    | 35:DA:826:U:O4'    | 2.12                     | 0.50              |
| 38:DD:35:LYS:CD    | 38:DD:36:PRO:N     | 2.63                     | 0.50              |
| 38:DD:43:ARG:HB3   | 38:DD:54:ARG:CB    | 2.40                     | 0.50              |
| 40:DF:160:ASN:HD21 | 40:DF:162:LEU:HD13 | 1.75                     | 0.50              |
| 40:DF:81:PRO:C     | 40:DF:83:PHE:H     | 2.15                     | 0.50              |
| 41:DG:179:PRO:O    | 41:DG:180:PHE:CD2  | 2.65                     | 0.50              |
| 41:DG:59:GLU:O     | 41:DG:62:LEU:HD13  | 2.11                     | 0.50              |
| 46:DN:48:MET:HE2   | 46:DN:48:MET:N     | 2.10                     | 0.50              |
| 52:DT:118:ARG:HA   | 52:DT:121:ILE:HD12 | 1.93                     | 0.50              |
| 58:DZ:56:VAL:HA    | 58:DZ:70:LEU:CD2   | 2.41                     | 0.50              |
| 1:AA:1348:U:H2'    | 1:AA:1349:A:C8     | 2.46                     | 0.50              |
| 1:AA:284:G:H2'     | 1:AA:285:G:H8      | 1.76                     | 0.50              |
| 1:AA:39:G:O2'      | 1:AA:40:C:H5'      | 2.11                     | 0.50              |
| 1:AA:489:C:H2'     | 1:AA:490:G:C8      | 2.46                     | 0.50              |
| 1:AA:637:G:O2'     | 1:AA:638:G:H5'     | 2.12                     | 0.50              |
| 1:AA:78:G:H1       | 1:AA:91:C:H42      | 1.60                     | 0.50              |
| 1:AA:867:G:O2'     | 1:AA:868:C:H5'     | 2.12                     | 0.50              |
| 2:AB:97:TRP:CH2    | 2:AB:176:GLU:CD    | 2.85                     | 0.50              |
| 4:AD:2:GLY:O       | 4:AD:4:TYR:N       | 2.45                     | 0.50              |
| 9:AI:128:ARG:O     | 13:AM:125:ARG:HD2  | 2.11                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:AJ:96:ILE:N     | 10:AJ:96:ILE:HD13  | 2.21                     | 0.50              |
| 12:AL:70:ILE:CG2   | 12:AL:100:ILE:HD12 | 2.41                     | 0.50              |
| 20:AT:11:SER:HA    | 20:AT:13:LEU:CD1   | 2.42                     | 0.50              |
| 20:AT:86:ARG:HH11  | 20:AT:86:ARG:HG3   | 1.77                     | 0.50              |
| 22:AV:29:G:C6      | 22:AV:30:G:N7      | 2.79                     | 0.50              |
| 22:AW:20:G:H4'     | 22:AW:21:U:OP2     | 2.10                     | 0.50              |
| 24:AY:20:HIS:N     | 24:AY:121:VAL:HG11 | 2.27                     | 0.50              |
| 24:AY:255:ILE:CG1  | 24:AY:256:THR:N    | 2.74                     | 0.50              |
| 24:AY:66:THR:O     | 24:AY:67:ALA:HB3   | 2.10                     | 0.50              |
| 26:B1:67:ILE:N     | 26:B1:68:PRO:HD2   | 2.26                     | 0.50              |
| 28:B3:31:LEU:HD22  | 28:B3:32:GLN:H     | 1.77                     | 0.50              |
| 29:B4:51:ASP:OD2   | 29:B4:52:THR:HG23  | 2.11                     | 0.50              |
| 33:B8:51:ALA:HA    | 33:B8:54:GLU:OE1   | 2.10                     | 0.50              |
| 35:BA:1288:U:H4'   | 35:BA:1289:C:OP2   | 2.11                     | 0.50              |
| 35:BA:1336:A:H2'   | 35:BA:1337:G:H8    | 1.76                     | 0.50              |
| 35:BA:2228:G:H2'   | 35:BA:2229:C:H6    | 1.77                     | 0.50              |
| 35:BA:2617:C:O2'   | 35:BA:2618:G:H5'   | 2.11                     | 0.50              |
| 30:B5:34:PRO:HG3   | 35:BA:2885:C:O2'   | 2.12                     | 0.50              |
| 35:BA:298:G:H8     | 35:BA:298:G:O5'    | 1.94                     | 0.50              |
| 35:BA:637:A:OP2    | 48:BP:115:LEU:HB2  | 2.12                     | 0.50              |
| 35:BA:705:A:C2     | 35:BA:727:A:H1'    | 2.47                     | 0.50              |
| 35:BA:817:C:H2'    | 35:BA:818:G:O4'    | 2.12                     | 0.50              |
| 35:BA:83:G:O2'     | 35:BA:84:A:C8      | 2.57                     | 0.50              |
| 39:BE:77:ILE:C     | 39:BE:78:LEU:HG    | 2.31                     | 0.50              |
| 40:BF:81:PRO:O     | 40:BF:83:PHE:N     | 2.45                     | 0.50              |
| 44:BK:93:ARG:HB2   | 58:BZ:112:ARG:CZ   | 2.42                     | 0.50              |
| 48:BP:102:ARG:HH21 | 48:BP:102:ARG:CB   | 2.25                     | 0.50              |
| 53:BU:79:PHE:CE2   | 53:BU:83:LEU:HD11  | 2.46                     | 0.50              |
| 57:BY:47:LYS:O     | 57:BY:48:ALA:O     | 2.30                     | 0.50              |
| 1:CA:1038:C:H2'    | 1:CA:1039:C:C6     | 2.47                     | 0.50              |
| 1:CA:1129:C:C6     | 1:CA:1129:C:H5'    | 2.45                     | 0.50              |
| 1:CA:1293:G:O2'    | 1:CA:1294:G:H5'    | 2.12                     | 0.50              |
| 1:CA:1301:U:H3'    | 1:CA:1302:U:H5''   | 1.93                     | 0.50              |
| 1:CA:1497:G:C2'    | 1:CA:1498:U:H5'    | 2.40                     | 0.50              |
| 1:CA:559:A:OP2     | 5:CE:126:ARG:NH2   | 2.44                     | 0.50              |
| 3:CC:90:GLU:HA     | 3:CC:93:LYS:CB     | 2.41                     | 0.50              |
| 10:CJ:47:PHE:CE2   | 14:CN:37:PHE:CE2   | 2.99                     | 0.50              |
| 15:CO:55:GLY:HA2   | 15:CO:58:MET:CE    | 2.40                     | 0.50              |
| 19:CS:15:LEU:O     | 19:CS:19:VAL:HB    | 2.12                     | 0.50              |
| 20:CT:84:LEU:O     | 20:CT:86:ARG:N     | 2.44                     | 0.50              |
| 22:CW:39:A:H2'     | 22:CW:40:C:O4'     | 2.12                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:CW:52:C:H2'     | 22:CW:53:G:C4'     | 2.42                     | 0.50              |
| 24:CY:400:GLU:HG2  | 24:CY:401:SER:N    | 2.26                     | 0.50              |
| 24:CY:590:ILE:HD13 | 24:CY:593:ALA:HB2  | 1.94                     | 0.50              |
| 24:CY:66:THR:O     | 24:CY:67:ALA:CB    | 2.60                     | 0.50              |
| 61:CY:702:FUA:C20  | 61:CY:702:FUA:H5   | 2.12                     | 0.50              |
| 31:D6:15:GLU:CD    | 31:D6:44:ARG:CZ    | 2.80                     | 0.50              |
| 35:DA:1015:G:H2'   | 35:DA:1016:G:H8    | 1.74                     | 0.50              |
| 35:DA:1420:U:H2'   | 35:DA:1421:G:H5'   | 1.93                     | 0.50              |
| 35:DA:1528:A:H2'   | 35:DA:1528:A:N3    | 2.26                     | 0.50              |
| 35:DA:1600:C:O2'   | 35:DA:1601:G:H5'   | 2.12                     | 0.50              |
| 35:DA:1610:A:H4'   | 35:DA:1611:C:OP2   | 2.11                     | 0.50              |
| 35:DA:2020:A:H2'   | 35:DA:2021:C:H5''  | 1.92                     | 0.50              |
| 35:DA:2886:G:H2'   | 35:DA:2887:U:H6    | 1.76                     | 0.50              |
| 35:DA:302:C:H2'    | 35:DA:303:U:C6     | 2.47                     | 0.50              |
| 35:DA:342:G:O2'    | 35:DA:343:C:H5'    | 2.12                     | 0.50              |
| 35:DA:532:A:H2'    | 35:DA:532:A:N3     | 2.27                     | 0.50              |
| 35:DA:259:G:N2     | 35:DA:621:A:H8     | 2.10                     | 0.50              |
| 35:DA:809:G:O2'    | 35:DA:810:U:H5'    | 2.12                     | 0.50              |
| 36:DB:85:G:O2'     | 36:DB:86:G:H5'     | 2.11                     | 0.50              |
| 38:DD:26:LYS:N     | 38:DD:26:LYS:HE2   | 2.26                     | 0.50              |
| 39:DE:188:VAL:HG23 | 39:DE:189:PRO:HD2  | 1.93                     | 0.50              |
| 35:DA:1035:U:O5'   | 42:DH:59:ARG:NH1   | 2.45                     | 0.50              |
| 43:DJ:13:UNK:C     | 43:DJ:15:UNK:N     | 2.73                     | 0.50              |
| 48:DP:25:SER:O     | 48:DP:30:THR:HG23  | 2.11                     | 0.50              |
| 52:DT:6:LEU:O      | 52:DT:9:LEU:N      | 2.45                     | 0.50              |
| 54:DV:99:ILE:HD13  | 54:DV:99:ILE:N     | 2.25                     | 0.50              |
| 55:DW:107:LEU:N    | 55:DW:107:LEU:HD22 | 2.26                     | 0.50              |
| 1:AA:1346:A:H1'    | 1:AA:1348:U:C5     | 2.47                     | 0.50              |
| 1:AA:1402:C:C5     | 1:AA:1403:C:C5     | 2.99                     | 0.50              |
| 1:AA:1459:C:H2'    | 1:AA:1460:A:C8     | 2.47                     | 0.50              |
| 1:AA:159:G:H2'     | 1:AA:160:A:H5''    | 1.94                     | 0.50              |
| 1:AA:177:C:C2      | 1:AA:178:C:C5      | 3.00                     | 0.50              |
| 1:AA:177:C:H2'     | 1:AA:178:C:H6      | 1.77                     | 0.50              |
| 1:AA:423:G:C2'     | 1:AA:424:G:H5'     | 2.41                     | 0.50              |
| 1:AA:452:A:O2'     | 1:AA:453:A:H8      | 1.94                     | 0.50              |
| 1:AA:80:G:H5''     | 1:AA:81:U:H5'      | 1.93                     | 0.50              |
| 1:AA:1205:U:O2'    | 3:AC:195:VAL:HG23  | 2.10                     | 0.50              |
| 6:AF:21:LEU:O      | 6:AF:25:ILE:HG12   | 2.11                     | 0.50              |
| 10:AJ:61:GLU:OE1   | 14:AN:49:HIS:CE1   | 2.61                     | 0.50              |
| 14:AN:25:VAL:HG23  | 14:AN:38:GLY:O     | 2.11                     | 0.50              |
| 17:AQ:94:ASN:O     | 17:AQ:96:GLU:N     | 2.45                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:AT:23:ARG:HA    | 20:AT:26:ASN:HD21  | 1.76                     | 0.50              |
| 22:AV:39:C:H2'     | 22:AV:40:C:H6      | 1.76                     | 0.50              |
| 24:AY:121:VAL:CA   | 24:AY:124:GLN:NE2  | 2.75                     | 0.50              |
| 24:AY:203:GLU:O    | 24:AY:204:GLU:O    | 2.28                     | 0.50              |
| 24:AY:132:ARG:O    | 24:AY:256:THR:HG23 | 2.11                     | 0.50              |
| 27:B2:50:ILE:O     | 27:B2:52:ASP:N     | 2.41                     | 0.50              |
| 29:B4:12:ALA:HB2   | 29:B4:29:PRO:HA    | 1.94                     | 0.50              |
| 35:BA:1156:A:O2'   | 35:BA:1157:G:OP1   | 2.30                     | 0.50              |
| 35:BA:2161:C:O2'   | 35:BA:2162:G:H5'   | 2.12                     | 0.50              |
| 25:B0:14:ARG:NH1   | 35:BA:2279:G:O6    | 2.45                     | 0.50              |
| 33:B8:31:HIS:HE1   | 35:BA:2392:A:OP2   | 1.94                     | 0.50              |
| 35:BA:532:A:N3     | 35:BA:532:A:H2'    | 2.26                     | 0.50              |
| 35:BA:756:C:C2'    | 35:BA:757:U:H5'    | 2.40                     | 0.50              |
| 37:BC:138:LEU:HD13 | 37:BC:138:LEU:C    | 2.32                     | 0.50              |
| 38:BD:14:ARG:HG3   | 38:BD:15:PHE:N     | 2.26                     | 0.50              |
| 38:BD:270:ILE:HD12 | 38:BD:270:ILE:O    | 2.11                     | 0.50              |
| 39:BE:69:LYS:HG2   | 39:BE:90:THR:OG1   | 2.11                     | 0.50              |
| 39:BE:93:VAL:C     | 39:BE:95:ILE:N     | 2.63                     | 0.50              |
| 42:BH:68:THR:C     | 42:BH:70:THR:H     | 2.15                     | 0.50              |
| 46:BN:133:GLN:CG   | 46:BN:134:ARG:N    | 2.75                     | 0.50              |
| 47:BO:20:MET:HE3   | 47:BO:44:LYS:HE3   | 1.93                     | 0.50              |
| 47:BO:32:TYR:N     | 47:BO:32:TYR:CD1   | 2.80                     | 0.50              |
| 48:BP:132:LYS:O    | 48:BP:136:GLU:HG2  | 2.10                     | 0.50              |
| 48:BP:7:ARG:HA     | 48:BP:7:ARG:NH1    | 2.26                     | 0.50              |
| 50:BR:48:VAL:O     | 50:BR:49:ASP:C     | 2.49                     | 0.50              |
| 51:BS:74:ALA:HB2   | 51:BS:101:LEU:CD2  | 2.41                     | 0.50              |
| 54:BV:99:ILE:H     | 54:BV:99:ILE:HD13  | 1.77                     | 0.50              |
| 35:BA:1614:A:N1    | 55:BW:91:GLY:HA2   | 2.27                     | 0.50              |
| 56:BX:57:LEU:HD13  | 56:BX:57:LEU:N     | 2.26                     | 0.50              |
| 58:BZ:54:HIS:CE1   | 58:BZ:123:ASP:OD2  | 2.63                     | 0.50              |
| 1:CA:1118:C:H42    | 1:CA:1155:G:H1     | 1.59                     | 0.50              |
| 1:CA:1303:C:N4     | 1:CA:1304:G:C6     | 2.80                     | 0.50              |
| 1:CA:1473:A:O2'    | 1:CA:1474:G:H5'    | 2.11                     | 0.50              |
| 1:CA:306:G:O2'     | 1:CA:307:C:H5'     | 2.12                     | 0.50              |
| 1:CA:703:G:O2'     | 1:CA:704:A:OP2     | 2.29                     | 0.50              |
| 5:CE:8:GLU:CA      | 5:CE:34:VAL:HG23   | 2.42                     | 0.50              |
| 6:CF:44:GLY:HA2    | 6:CF:59:TYR:CE1    | 2.46                     | 0.50              |
| 8:CH:6:ILE:H       | 8:CH:6:ILE:HD12    | 1.77                     | 0.50              |
| 8:CH:86:ILE:HG13   | 8:CH:133:LEU:HD22  | 1.92                     | 0.50              |
| 16:CP:60:LEU:HD21  | 16:CP:66:PRO:HD3   | 1.92                     | 0.50              |
| 24:CY:415:PRO:O    | 24:CY:416:LYS:C    | 2.50                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:CY:439:ARG:O    | 24:CY:452:SER:CB   | 2.60                     | 0.50              |
| 35:DA:1316:U:O2'   | 35:DA:1317:A:H5'   | 2.11                     | 0.50              |
| 35:DA:1536:C:H2'   | 35:DA:1537:G:H4'   | 1.93                     | 0.50              |
| 35:DA:1567:A:H5'   | 38:DD:58:HIS:CD2   | 2.46                     | 0.50              |
| 35:DA:1719:G:H2'   | 35:DA:1720:U:H5'   | 1.94                     | 0.50              |
| 35:DA:1853:A:H2'   | 35:DA:1854:A:C8    | 2.47                     | 0.50              |
| 35:DA:2415:G:H2'   | 35:DA:2416:C:C6    | 2.47                     | 0.50              |
| 35:DA:1669:A:H4'   | 35:DA:2549:G:H4'   | 1.94                     | 0.50              |
| 35:DA:346:A:N3     | 35:DA:346:A:H2'    | 2.25                     | 0.50              |
| 35:DA:600:G:H2'    | 35:DA:601:C:C6     | 2.47                     | 0.50              |
| 35:DA:750:A:H3'    | 35:DA:751:A:H5''   | 1.94                     | 0.50              |
| 35:DA:945:A:C2     | 35:DA:2448:A:N1    | 2.80                     | 0.50              |
| 36:DB:81:G:H2'     | 36:DB:82:G:H5'     | 1.93                     | 0.50              |
| 38:DD:43:ARG:CB    | 38:DD:54:ARG:HB2   | 2.39                     | 0.50              |
| 38:DD:39:LYS:HZ1   | 38:DD:87:ASN:HB3   | 1.74                     | 0.50              |
| 35:DA:2810:A:H2'   | 39:DE:61:ARG:NH2   | 2.26                     | 0.50              |
| 41:DG:114:ILE:O    | 41:DG:114:ILE:HG22 | 2.12                     | 0.50              |
| 48:DP:132:LYS:O    | 48:DP:136:GLU:HG2  | 2.11                     | 0.50              |
| 49:DQ:110:THR:CG2  | 49:DQ:113:GLN:HG3  | 2.42                     | 0.50              |
| 56:DX:57:LEU:HD13  | 56:DX:57:LEU:N     | 2.27                     | 0.50              |
| 58:DZ:12:GLY:HA2   | 58:DZ:36:LYS:HZ3   | 1.77                     | 0.50              |
| 58:DZ:154:ASP:N    | 58:DZ:154:ASP:OD2  | 2.44                     | 0.50              |
| 58:DZ:171:ILE:HG13 | 58:DZ:172:ALA:H    | 1.76                     | 0.50              |
| 1:AA:1430:C:H6     | 1:AA:1430:C:O5'    | 1.95                     | 0.50              |
| 1:AA:404:U:H2'     | 1:AA:405:U:C6      | 2.47                     | 0.50              |
| 1:AA:6:G:H2'       | 5:AE:119:LEU:CD1   | 2.42                     | 0.50              |
| 1:AA:895:G:H5''    | 1:AA:896:C:OP2     | 2.11                     | 0.50              |
| 1:AA:950:U:H2'     | 1:AA:951:G:C8      | 2.45                     | 0.50              |
| 1:AA:957:U:H2'     | 1:AA:959:A:OP2     | 2.12                     | 0.50              |
| 2:AB:91:PRO:HG2    | 2:AB:155:LEU:HD23  | 1.94                     | 0.50              |
| 3:AC:90:GLU:HA     | 3:AC:93:LYS:CB     | 2.41                     | 0.50              |
| 4:AD:61:LYS:NZ     | 4:AD:72:GLU:OE2    | 2.42                     | 0.50              |
| 12:AL:115:LYS:O    | 12:AL:117:ARG:N    | 2.45                     | 0.50              |
| 10:AJ:47:PHE:CE2   | 14:AN:37:PHE:CE2   | 3.00                     | 0.50              |
| 15:AO:43:LEU:HD12  | 15:AO:56:LEU:HD22  | 1.93                     | 0.50              |
| 24:AY:204:GLU:H    | 24:AY:204:GLU:CD   | 2.14                     | 0.50              |
| 24:AY:388:THR:CG2  | 24:AY:399:LEU:HD13 | 2.42                     | 0.50              |
| 24:AY:415:PRO:HG3  | 24:AY:421:GLN:HG2  | 1.94                     | 0.50              |
| 24:AY:481:VAL:HG23 | 24:AY:483:TYR:CE2  | 2.47                     | 0.50              |
| 24:AY:655:TYR:CZ   | 24:AY:659:LEU:HD23 | 2.47                     | 0.50              |
| 24:AY:679:VAL:HB   | 24:AY:683:VAL:HB   | 1.94                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:1168:G:H2'   | 35:BA:1169:G:O4'   | 2.12                     | 0.50              |
| 35:BA:1301:A:HO2'  | 35:BA:1302:A:P     | 2.34                     | 0.50              |
| 35:BA:1829:A:N3    | 38:BD:15:PHE:CZ    | 2.80                     | 0.50              |
| 35:BA:2733:A:O2'   | 35:BA:2734:A:H5'   | 2.12                     | 0.50              |
| 35:BA:803:U:H2'    | 35:BA:804:A:H5'    | 1.92                     | 0.50              |
| 36:BB:13:A:O2'     | 36:BB:15:A:H5''    | 2.11                     | 0.50              |
| 37:BC:4:HIS:HB3    | 37:BC:8:TYR:HD2    | 1.77                     | 0.50              |
| 38:BD:200:ASP:O    | 38:BD:201:HIS:C    | 2.50                     | 0.50              |
| 38:BD:26:LYS:O     | 38:BD:27:THR:CB    | 2.60                     | 0.50              |
| 39:BE:14:ILE:HG13  | 39:BE:21:VAL:CG2   | 2.41                     | 0.50              |
| 40:BF:41:LEU:HD23  | 40:BF:44:ARG:HE    | 1.77                     | 0.50              |
| 41:BG:61:ALA:HB2   | 41:BG:68:PRO:HD3   | 1.94                     | 0.50              |
| 42:BH:29:PRO:HD2   | 42:BH:79:VAL:O     | 2.12                     | 0.50              |
| 35:BA:1064:C:H4'   | 44:BK:89:HIS:CD2   | 2.46                     | 0.50              |
| 46:BN:23:LEU:HB3   | 46:BN:60:ILE:CG2   | 2.39                     | 0.50              |
| 49:BQ:110:THR:HG22 | 49:BQ:113:GLN:OE1  | 2.11                     | 0.50              |
| 49:BQ:17:LEU:O     | 49:BQ:18:LYS:HD2   | 2.12                     | 0.50              |
| 49:BQ:41:TRP:HE1   | 49:BQ:96:VAL:HG22  | 1.76                     | 0.50              |
| 54:BV:5:VAL:HG23   | 54:BV:37:VAL:HG23  | 1.93                     | 0.50              |
| 58:BZ:67:LEU:HD23  | 58:BZ:90:VAL:HG11  | 1.93                     | 0.50              |
| 1:CA:1222:G:O2'    | 1:CA:1223:C:H5'    | 2.11                     | 0.50              |
| 1:CA:1277:C:H6     | 1:CA:1277:C:H3'    | 1.77                     | 0.50              |
| 1:CA:429:U:H4'     | 1:CA:430:A:O5'     | 2.11                     | 0.50              |
| 1:CA:538:G:OP2     | 12:CL:115:LYS:HG3  | 2.11                     | 0.50              |
| 1:CA:622:A:C8      | 1:CA:623:C:C5      | 2.99                     | 0.50              |
| 2:CB:211:ILE:HG22  | 2:CB:215:LEU:HD23  | 1.93                     | 0.50              |
| 2:CB:223:ILE:HG23  | 2:CB:226:ARG:HD2   | 1.93                     | 0.50              |
| 3:CC:54:ARG:HH11   | 3:CC:54:ARG:HG2    | 1.76                     | 0.50              |
| 1:CA:1147:C:O2'    | 9:CI:16:ARG:HD2    | 2.11                     | 0.50              |
| 14:CN:12:ARG:O     | 14:CN:14:PRO:CD    | 2.59                     | 0.50              |
| 22:CW:11:A:H61     | 22:CW:25:U:H3      | 1.59                     | 0.50              |
| 22:CW:53:G:O6      | 22:CW:63:C:N3      | 2.45                     | 0.50              |
| 24:CY:122:TRP:O    | 24:CY:125:ALA:N    | 2.31                     | 0.50              |
| 24:CY:177:ILE:C    | 24:CY:178:ILE:HD12 | 2.32                     | 0.50              |
| 26:D1:23:LYS:HE2   | 26:D1:28:GLY:CA    | 2.30                     | 0.50              |
| 26:D1:26:ARG:HG3   | 26:D1:27:GLU:N     | 2.26                     | 0.50              |
| 27:D2:21:LEU:O     | 27:D2:25:VAL:HG23  | 2.11                     | 0.50              |
| 35:DA:1043:C:H2'   | 35:DA:1044:G:C5'   | 2.19                     | 0.50              |
| 35:DA:1240:U:O2'   | 35:DA:1241:A:H5'   | 2.10                     | 0.50              |
| 35:DA:582:G:C6     | 35:DA:1259:G:N1    | 2.80                     | 0.50              |
| 35:DA:1344:G:H1    | 35:DA:1403:C:H42   | 1.60                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:1528:A:C2    | 35:DA:1542:A:H2    | 2.29                     | 0.50              |
| 35:DA:1930:G:N2    | 35:DA:1968:G:H2'   | 2.27                     | 0.50              |
| 35:DA:2337:G:H2'   | 35:DA:2338:G:H8    | 1.77                     | 0.50              |
| 35:DA:2853:C:H2'   | 35:DA:2854:G:H8    | 1.76                     | 0.50              |
| 35:DA:737:C:H2'    | 35:DA:738:G:H5'    | 1.93                     | 0.50              |
| 27:D2:59:ARG:HA    | 35:DA:76:C:O2'     | 2.11                     | 0.50              |
| 42:DH:37:VAL:CG1   | 42:DH:38:SER:N     | 2.75                     | 0.50              |
| 44:DK:95:LYS:HG2   | 44:DK:137:GLU:OE1  | 2.11                     | 0.50              |
| 46:DN:15:LEU:HD23  | 46:DN:53:VAL:HB    | 1.94                     | 0.50              |
| 48:DP:101:VAL:HB   | 48:DP:107:LYS:HA   | 1.94                     | 0.50              |
| 35:DA:636:G:H2'    | 48:DP:115:LEU:HD12 | 1.93                     | 0.50              |
| 52:DT:56:GLY:O     | 52:DT:59:THR:HG23  | 2.11                     | 0.50              |
| 53:DU:13:LYS:O     | 53:DU:16:LYS:HB2   | 2.12                     | 0.50              |
| 56:DX:10:ALA:HB1   | 56:DX:11:PRO:CD    | 2.41                     | 0.50              |
| 27:D2:29:LYS:NZ    | 56:DX:6:ASP:OD2    | 2.41                     | 0.50              |
| 58:DZ:128:VAL:CG2  | 58:DZ:129:SER:N    | 2.73                     | 0.50              |
| 1:AA:1202:G:C2'    | 1:AA:1203:C:H5'    | 2.42                     | 0.50              |
| 1:AA:174:C:H2'     | 1:AA:175:C:H6      | 1.75                     | 0.50              |
| 1:AA:141:A:H1'     | 1:AA:182:U:C2      | 2.47                     | 0.50              |
| 1:AA:555:C:H2'     | 1:AA:556:C:C6      | 2.47                     | 0.50              |
| 3:AC:28:GLN:O      | 3:AC:29:TYR:C      | 2.50                     | 0.50              |
| 1:AA:620:C:C2      | 4:AD:135:LEU:HG    | 2.47                     | 0.50              |
| 5:AE:43:LEU:CD2    | 5:AE:132:ALA:HB1   | 2.41                     | 0.50              |
| 5:AE:142:LEU:O     | 5:AE:143:ARG:NE    | 2.42                     | 0.50              |
| 18:AR:87:ARG:CB    | 18:AR:87:ARG:HH11  | 2.25                     | 0.50              |
| 19:AS:41:VAL:CG2   | 19:AS:44:MET:HB2   | 2.35                     | 0.50              |
| 22:AV:20:U:C3'     | 22:AV:21:A:C5'     | 2.90                     | 0.50              |
| 24:AY:177:ILE:HG22 | 24:AY:178:ILE:H    | 1.77                     | 0.50              |
| 24:AY:181:LEU:HD12 | 24:AY:242:LEU:HD13 | 1.94                     | 0.50              |
| 24:AY:264:LEU:HD23 | 24:AY:264:LEU:C    | 2.33                     | 0.50              |
| 24:AY:628:ARG:HH11 | 24:AY:628:ARG:HG2  | 1.77                     | 0.50              |
| 24:AY:74:TRP:CH2   | 24:AY:270:GLN:HG2  | 2.47                     | 0.50              |
| 27:B2:3:LEU:HD22   | 27:B2:7:ARG:HH22   | 1.76                     | 0.50              |
| 29:B4:14:ILE:HG22  | 29:B4:15:ILE:N     | 2.27                     | 0.50              |
| 31:B6:6:ARG:C      | 31:B6:8:LYS:H      | 2.15                     | 0.50              |
| 35:BA:1142(A):A:C5 | 35:BA:1144:G:C5    | 3.00                     | 0.50              |
| 35:BA:1623:G:H2'   | 35:BA:1624:G:H8    | 1.77                     | 0.50              |
| 35:BA:781:A:H2'    | 35:BA:1777:U:O2'   | 2.11                     | 0.50              |
| 35:BA:1827:C:H2'   | 35:BA:1828:G:O4'   | 2.11                     | 0.50              |
| 35:BA:2307:G:H3'   | 35:BA:2307:G:N3    | 2.27                     | 0.50              |
| 35:BA:2348:U:C2'   | 35:BA:2349:G:C5'   | 2.88                     | 0.50              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:2892:A:H62   | 35:BA:2893:G:H21   | 1.59                     | 0.50              |
| 35:BA:760:G:C2'    | 35:BA:761:A:H5'    | 2.41                     | 0.50              |
| 36:BB:15:A:C3'     | 36:BB:16:G:H5'     | 2.42                     | 0.50              |
| 37:BC:60:ARG:HG2   | 37:BC:61:GLY:N     | 2.26                     | 0.50              |
| 39:BE:9:VAL:HG22   | 39:BE:10:GLY:N     | 2.26                     | 0.50              |
| 40:BF:160:ASN:HD21 | 40:BF:162:LEU:HD13 | 1.76                     | 0.50              |
| 40:BF:170:LEU:N    | 40:BF:170:LEU:HD22 | 2.27                     | 0.50              |
| 41:BG:98:ARG:H     | 41:BG:98:ARG:NH1   | 2.07                     | 0.50              |
| 42:BH:50:VAL:HG12  | 42:BH:51:ARG:N     | 2.26                     | 0.50              |
| 44:BK:95:LYS:HG2   | 44:BK:137:GLU:OE1  | 2.11                     | 0.50              |
| 46:BN:2:LYS:O      | 46:BN:4:TYR:CZ     | 2.65                     | 0.50              |
| 48:BP:140:ALA:O    | 48:BP:141:ALA:HB3  | 2.12                     | 0.50              |
| 53:BU:83:LEU:N     | 53:BU:83:LEU:CD1   | 2.72                     | 0.50              |
| 54:BV:35:LEU:C     | 54:BV:37:VAL:N     | 2.64                     | 0.50              |
| 58:BZ:143:GLY:C    | 58:BZ:144:LEU:HD22 | 2.32                     | 0.50              |
| 58:BZ:9:TYR:HB3    | 58:BZ:35:ARG:HH22  | 1.77                     | 0.50              |
| 1:CA:1122:U:C2'    | 1:CA:1123:A:H5'    | 2.42                     | 0.50              |
| 3:CC:128:PHE:O     | 3:CC:130:VAL:N     | 2.45                     | 0.50              |
| 4:CD:101:LEU:HD23  | 4:CD:121:VAL:HG13  | 1.94                     | 0.50              |
| 6:CF:67:MET:HB2    | 6:CF:68:PRO:CD     | 2.37                     | 0.50              |
| 9:CI:5:TYR:HD2     | 9:CI:17:VAL:O      | 1.94                     | 0.50              |
| 9:CI:93:ARG:HA     | 9:CI:96:LEU:HB2    | 1.94                     | 0.50              |
| 13:CM:54:VAL:O     | 13:CM:56:LEU:N     | 2.45                     | 0.50              |
| 28:D3:54:VAL:HG12  | 28:D3:55:ARG:N     | 2.27                     | 0.50              |
| 30:D5:48:GLU:O     | 30:D5:49:CYS:HB3   | 2.12                     | 0.50              |
| 31:D6:27:LYS:HB3   | 31:D6:32:ASN:HD22  | 1.75                     | 0.50              |
| 31:D6:47:THR:CG2   | 31:D6:48:VAL:H     | 2.19                     | 0.50              |
| 35:DA:1317:A:H2'   | 35:DA:1318:C:C6    | 2.47                     | 0.50              |
| 35:DA:1437:C:H2'   | 35:DA:1438:U:C6    | 2.46                     | 0.50              |
| 35:DA:1784:A:H4'   | 35:DA:1785:A:O5'   | 2.10                     | 0.50              |
| 35:DA:1998:G:O2'   | 35:DA:1999:C:H5'   | 2.12                     | 0.50              |
| 35:DA:2695:C:H2'   | 35:DA:2696:U:C6    | 2.47                     | 0.50              |
| 35:DA:2705:A:H2'   | 35:DA:2706:G:O4'   | 2.12                     | 0.50              |
| 35:DA:274:G:N3     | 35:DA:274:G:C2'    | 2.74                     | 0.50              |
| 35:DA:664:C:O2'    | 35:DA:665:C:H5'    | 2.10                     | 0.50              |
| 35:DA:71:A:H4'     | 35:DA:72:U:H5''    | 1.93                     | 0.50              |
| 35:DA:811:U:H3'    | 35:DA:812:C:C5'    | 2.41                     | 0.50              |
| 35:DA:827:U:H2'    | 35:DA:2068:U:O2    | 2.12                     | 0.50              |
| 35:DA:852:G:H2'    | 35:DA:853:G:C8     | 2.46                     | 0.50              |
| 38:DD:24:ILE:CG1   | 38:DD:25:THR:N     | 2.75                     | 0.50              |
| 39:DE:69:LYS:HG2   | 39:DE:90:THR:OG1   | 2.12                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:DF:100:THR:O    | 40:DF:100:THR:HG22 | 2.12                     | 0.50              |
| 41:DG:88:ILE:HG23  | 41:DG:89:GLY:N     | 2.27                     | 0.50              |
| 42:DH:149:ARG:HA   | 42:DH:162:ILE:HG13 | 1.92                     | 0.50              |
| 46:DN:2:LYS:O      | 46:DN:4:TYR:CZ     | 2.64                     | 0.50              |
| 48:DP:89:ALA:HA    | 48:DP:121:LYS:HD3  | 1.93                     | 0.50              |
| 48:DP:112:LEU:N    | 48:DP:128:HIS:HD2  | 2.09                     | 0.50              |
| 49:DQ:109:VAL:HG12 | 49:DQ:113:GLN:HB2  | 1.94                     | 0.50              |
| 50:DR:100:LEU:HD13 | 50:DR:100:LEU:N    | 2.26                     | 0.50              |
| 50:DR:10:LEU:CD2   | 50:DR:17:ARG:HD3   | 2.42                     | 0.50              |
| 50:DR:26:LYS:CE    | 50:DR:71:GLN:H     | 2.25                     | 0.50              |
| 53:DU:47:TYR:CA    | 53:DU:50:ARG:NH2   | 2.73                     | 0.50              |
| 56:DX:35:THR:HG22  | 56:DX:36:LYS:N     | 2.27                     | 0.50              |
| 58:DZ:35:ARG:CG    | 58:DZ:35:ARG:HH11  | 2.25                     | 0.50              |
| 1:AA:1288:A:H2'    | 1:AA:1289:A:C8     | 2.47                     | 0.50              |
| 1:AA:1511:G:O2'    | 1:AA:1512:U:H5'    | 2.11                     | 0.50              |
| 1:AA:375:U:C2      | 1:AA:376:G:C8      | 2.99                     | 0.50              |
| 1:AA:489:C:H2'     | 1:AA:490:G:H8      | 1.76                     | 0.50              |
| 1:AA:505:G:H5'     | 1:AA:534:U:H2'     | 1.94                     | 0.50              |
| 1:AA:940:C:O2'     | 1:AA:941:G:H5'     | 2.12                     | 0.50              |
| 2:AB:189:ASP:C     | 2:AB:191:ASP:H     | 2.15                     | 0.50              |
| 2:AB:51:LEU:CD2    | 2:AB:55:PHE:HE2    | 2.24                     | 0.50              |
| 3:AC:94:LEU:O      | 3:AC:94:LEU:HD12   | 2.11                     | 0.50              |
| 18:AR:53:ARG:C     | 18:AR:55:ARG:N     | 2.63                     | 0.50              |
| 24:AY:115:GLU:HG3  | 24:AY:115:GLU:O    | 2.12                     | 0.50              |
| 26:B1:76:ARG:CZ    | 26:B1:95:LEU:HD22  | 2.41                     | 0.50              |
| 35:BA:1052:C:O2'   | 35:BA:1053:C:O5'   | 2.30                     | 0.50              |
| 35:BA:1071:G:N2    | 35:BA:1090:U:C5    | 2.80                     | 0.50              |
| 35:BA:1186:G:C2'   | 35:BA:1187:G:H5'   | 2.42                     | 0.50              |
| 22:AW:20:G:C5      | 35:BA:2169:A:H2    | 2.29                     | 0.50              |
| 35:BA:2307:G:H21   | 35:BA:2308:G:C5'   | 2.25                     | 0.50              |
| 35:BA:2853:C:H2'   | 35:BA:2854:G:C8    | 2.46                     | 0.50              |
| 35:BA:483:A:H2'    | 35:BA:483:A:N3     | 2.26                     | 0.50              |
| 35:BA:259:G:N2     | 35:BA:621:A:H8     | 2.09                     | 0.50              |
| 38:BD:78:LYS:HG2   | 38:BD:79:VAL:N     | 2.27                     | 0.50              |
| 40:BF:180:GLY:O    | 40:BF:182:ASN:N    | 2.45                     | 0.50              |
| 40:BF:42:ALA:O     | 40:BF:45:ARG:HG3   | 2.12                     | 0.50              |
| 44:BK:100:THR:OG1  | 44:BK:103:GLN:HG3  | 2.12                     | 0.50              |
| 44:BK:13:PRO:HA    | 44:BK:52:ILE:HA    | 1.94                     | 0.50              |
| 47:BO:64:ARG:NH1   | 47:BO:83:ALA:HB2   | 2.27                     | 0.50              |
| 48:BP:101:VAL:HB   | 48:BP:107:LYS:HA   | 1.93                     | 0.50              |
| 50:BR:7:GLY:HA3    | 50:BR:8:ARG:NH2    | 2.27                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:BS:17:ARG:HA    | 51:BS:20:ARG:NH1   | 2.27                     | 0.50              |
| 35:BA:2019:A:O4'   | 53:BU:34:LYS:HD2   | 2.12                     | 0.50              |
| 54:BV:46:VAL:HG13  | 54:BV:47:VAL:N     | 2.27                     | 0.50              |
| 55:BW:14:PRO:HG2   | 55:BW:78:GLU:HB2   | 1.94                     | 0.50              |
| 1:CA:1125:U:H2'    | 1:CA:1126:U:H2'    | 1.94                     | 0.50              |
| 1:CA:1286:A:H2'    | 1:CA:1287:A:H4'    | 1.94                     | 0.50              |
| 1:CA:1490:C:H2'    | 1:CA:1491:G:C5'    | 2.41                     | 0.50              |
| 1:CA:238:G:C6      | 1:CA:239:U:C4      | 3.00                     | 0.50              |
| 1:CA:509:A:H5'     | 1:CA:510:A:P       | 2.50                     | 0.50              |
| 1:CA:1205:U:O2'    | 3:CC:195:VAL:HG23  | 2.12                     | 0.50              |
| 4:CD:4:TYR:O       | 4:CD:5:ILE:CB      | 2.59                     | 0.50              |
| 5:CE:12:LEU:HD13   | 5:CE:12:LEU:O      | 2.12                     | 0.50              |
| 5:CE:72:GLN:O      | 5:CE:73:ASN:HB2    | 2.11                     | 0.50              |
| 7:CG:29:LYS:HB2    | 7:CG:105:VAL:HG21  | 1.94                     | 0.50              |
| 10:CJ:50:ILE:HD13  | 10:CJ:50:ILE:N     | 2.16                     | 0.50              |
| 12:CL:79:GLU:HB2   | 24:CY:442:THR:CG2  | 2.35                     | 0.50              |
| 13:CM:65:LYS:C     | 13:CM:66:LEU:HD12  | 2.32                     | 0.50              |
| 14:CN:15:LYS:O     | 14:CN:16:PHE:C     | 2.50                     | 0.50              |
| 20:CT:26:ASN:N     | 20:CT:26:ASN:ND2   | 2.59                     | 0.50              |
| 22:CV:35:A:HO2'    | 22:CV:36:U:H5'     | 1.75                     | 0.50              |
| 24:CY:119:GLU:O    | 24:CY:121:VAL:N    | 2.43                     | 0.50              |
| 24:CY:137:ASN:ND2  | 24:CY:263:ALA:H    | 2.10                     | 0.50              |
| 24:CY:441:SER:O    | 24:CY:449:THR:HG23 | 2.12                     | 0.50              |
| 24:CY:65:ILE:H     | 24:CY:65:ILE:HD13  | 1.77                     | 0.50              |
| 30:D5:16:ARG:HD2   | 30:D5:20:ARG:HH12  | 1.77                     | 0.50              |
| 35:DA:1142(A):A:C5 | 35:DA:1144:G:C5    | 3.00                     | 0.50              |
| 35:DA:1145:C:H2'   | 35:DA:1146:C:H6    | 1.77                     | 0.50              |
| 35:DA:999:U:H5''   | 35:DA:1154:G:O6    | 2.12                     | 0.50              |
| 35:DA:1491:G:O2'   | 38:DD:101:GLU:HB2  | 2.12                     | 0.50              |
| 35:DA:1623:G:H2'   | 35:DA:1624:G:H8    | 1.77                     | 0.50              |
| 35:DA:1722:A:H2    | 35:DA:1740:G:H2'   | 1.77                     | 0.50              |
| 35:DA:1972:A:H2'   | 35:DA:1973:G:C8    | 2.46                     | 0.50              |
| 35:DA:2453:A:H2'   | 35:DA:2454:G:C8    | 2.46                     | 0.50              |
| 35:DA:2521:C:N4    | 35:DA:2544:G:H1    | 2.07                     | 0.50              |
| 35:DA:74:A:O2'     | 35:DA:75:G:OP2     | 2.28                     | 0.50              |
| 37:DC:4:HIS:HB3    | 37:DC:8:TYR:HD2    | 1.77                     | 0.50              |
| 38:DD:176:ARG:CG   | 38:DD:176:ARG:HH11 | 2.24                     | 0.50              |
| 38:DD:210:GLY:O    | 38:DD:211:ARG:CB   | 2.60                     | 0.50              |
| 39:DE:9:VAL:HG22   | 39:DE:10:GLY:N     | 2.25                     | 0.50              |
| 39:DE:32:PRO:N     | 39:DE:90:THR:HG23  | 2.27                     | 0.50              |
| 39:DE:50:GLY:CA    | 39:DE:78:LEU:HB3   | 2.40                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:DE:81:ILE:CG2   | 39:DE:81:ILE:O     | 2.59                     | 0.50              |
| 29:D4:25:TYR:O     | 41:DG:105:LYS:NZ   | 2.45                     | 0.50              |
| 41:DG:77:ILE:CG2   | 41:DG:80:PHE:N     | 2.74                     | 0.50              |
| 49:DQ:62:GLY:HA2   | 58:DZ:116:VAL:CG2  | 2.41                     | 0.50              |
| 51:DS:14:VAL:O     | 51:DS:15:ARG:C     | 2.47                     | 0.50              |
| 53:DU:112:ARG:CG   | 53:DU:112:ARG:HH11 | 2.25                     | 0.50              |
| 58:DZ:102:LEU:HD11 | 58:DZ:124:ILE:HG21 | 1.93                     | 0.50              |
| 58:DZ:142:SER:N    | 58:DZ:144:LEU:HD23 | 2.26                     | 0.50              |
| 58:DZ:152:ALA:HB3  | 58:DZ:154:ASP:OD2  | 2.12                     | 0.50              |
| 58:DZ:70:LEU:HG    | 58:DZ:91:LEU:CD1   | 2.42                     | 0.50              |
| 1:AA:1346:A:N6     | 1:AA:1375:A:OP2    | 2.41                     | 0.49              |
| 1:AA:193:C:H2'     | 1:AA:194:C:C6      | 2.47                     | 0.49              |
| 1:AA:429:U:H4'     | 1:AA:430:A:O5'     | 2.11                     | 0.49              |
| 1:AA:737:A:H2'     | 1:AA:738:C:H6      | 1.74                     | 0.49              |
| 1:AA:765:G:H22     | 1:AA:812:C:HO2'    | 1.58                     | 0.49              |
| 3:AC:5:ILE:CD1     | 3:AC:5:ILE:H       | 2.25                     | 0.49              |
| 5:AE:12:LEU:HD13   | 5:AE:12:LEU:O      | 2.12                     | 0.49              |
| 9:AI:40:LEU:O      | 9:AI:42:ARG:N      | 2.41                     | 0.49              |
| 12:AL:47:LYS:CB    | 12:AL:48:PRO:CD    | 2.89                     | 0.49              |
| 12:AL:92:ASP:O     | 12:AL:94:PRO:HD3   | 2.12                     | 0.49              |
| 13:AM:78:ILE:CA    | 13:AM:81:LEU:HD23  | 2.40                     | 0.49              |
| 1:AA:376:G:OP2     | 16:AP:67:THR:HG21  | 2.12                     | 0.49              |
| 22:AV:28:C:H2'     | 22:AV:29:G:C8      | 2.47                     | 0.49              |
| 24:AY:223:PHE:CE2  | 24:AY:249:GLY:HA3  | 2.47                     | 0.49              |
| 24:AY:337:SER:HA   | 24:AY:355:LEU:CD2  | 2.42                     | 0.49              |
| 24:AY:525:PHE:N    | 24:AY:525:PHE:CD1  | 2.80                     | 0.49              |
| 24:AY:92:ILE:CG2   | 24:AY:93:GLU:N     | 2.74                     | 0.49              |
| 27:B2:2:LYS:HB3    | 35:BA:97:C:H5''    | 1.94                     | 0.49              |
| 29:B4:19:GLY:O     | 29:B4:20:ASN:C     | 2.51                     | 0.49              |
| 30:B5:42:PRO:HB2   | 30:B5:43:HIS:CD2   | 2.47                     | 0.49              |
| 31:B6:28:ARG:O     | 31:B6:32:ASN:HB2   | 2.11                     | 0.49              |
| 31:B6:43:CYS:O     | 31:B6:44:ARG:NE    | 2.45                     | 0.49              |
| 35:BA:1336:A:OP2   | 56:BX:64:LYS:HE3   | 2.11                     | 0.49              |
| 35:BA:1558:A:O2'   | 35:BA:1559:G:OP2   | 2.29                     | 0.49              |
| 35:BA:1668:A:H61   | 35:BA:1676:A:H61   | 1.59                     | 0.49              |
| 35:BA:2028:U:H2'   | 35:BA:2029:G:C8    | 2.47                     | 0.49              |
| 35:BA:2062:A:N3    | 35:BA:2062:A:O4'   | 2.45                     | 0.49              |
| 35:BA:2502:G:H5''  | 35:BA:2503:A:C5'   | 2.37                     | 0.49              |
| 35:BA:302:C:H2'    | 35:BA:303:U:H6     | 1.77                     | 0.49              |
| 35:BA:342:G:O2'    | 35:BA:343:C:H5'    | 2.12                     | 0.49              |
| 35:BA:802:A:H2'    | 35:BA:803:U:C6     | 2.47                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:B2:47:ASN:HD22 | 35:BA:94(A):G:H21  | 1.59                     | 0.49              |
| 37:BC:135:ARG:HD2 | 37:BC:135:ARG:N    | 2.27                     | 0.49              |
| 38:BD:227:ASN:HB3 | 38:BD:228:PRO:HD2  | 1.93                     | 0.49              |
| 35:BA:1567:A:C5'  | 38:BD:58:HIS:CD2   | 2.95                     | 0.49              |
| 38:BD:73:VAL:O    | 38:BD:75:ILE:HG12  | 2.11                     | 0.49              |
| 39:BE:36:ARG:NH2  | 39:BE:88:GLY:CA    | 2.74                     | 0.49              |
| 40:BF:168:ARG:C   | 40:BF:170:LEU:H    | 2.16                     | 0.49              |
| 43:BJ:26:UNK:CB   | 43:BJ:84:UNK:HA    | 2.41                     | 0.49              |
| 48:BP:108:LYS:C   | 48:BP:110:TYR:N    | 2.64                     | 0.49              |
| 48:BP:16:ARG:HD3  | 48:BP:18:ARG:N     | 2.11                     | 0.49              |
| 49:BQ:67:ARG:HD2  | 49:BQ:105:GLU:OE1  | 2.12                     | 0.49              |
| 50:BR:4:LEU:C     | 50:BR:6:SER:N      | 2.64                     | 0.49              |
| 53:BU:26:GLY:C    | 53:BU:28:ARG:H     | 2.16                     | 0.49              |
| 53:BU:92:ARG:CD   | 53:BU:94:ASN:HB3   | 2.41                     | 0.49              |
| 54:BV:2:PHE:O     | 54:BV:14:VAL:O     | 2.30                     | 0.49              |
| 1:CA:1377:A:H2'   | 7:CG:7:ALA:HB2     | 1.94                     | 0.49              |
| 1:CA:318:G:H2'    | 1:CA:319:G:H8      | 1.76                     | 0.49              |
| 1:CA:66:G:C4'     | 1:CA:173:U:C5      | 2.95                     | 0.49              |
| 1:CA:719:C:O2'    | 18:CR:49:LYS:HB3   | 2.12                     | 0.49              |
| 4:CD:170:VAL:O    | 4:CD:171:GLY:O     | 2.30                     | 0.49              |
| 7:CG:65:ALA:HA    | 7:CG:128:ALA:HA    | 1.94                     | 0.49              |
| 9:CI:83:ARG:O     | 9:CI:86:VAL:HG12   | 2.12                     | 0.49              |
| 22:CV:19:G:H3'    | 22:CV:20:U:O2      | 2.12                     | 0.49              |
| 22:CV:23:C:H2'    | 22:CV:24:U:C6      | 2.46                     | 0.49              |
| 24:CY:678:GLU:CG  | 24:CY:679:VAL:N    | 2.74                     | 0.49              |
| 32:D7:46:VAL:CG1  | 32:D7:47:ARG:N     | 2.73                     | 0.49              |
| 35:DA:1264:G:O3'  | 35:DA:2615:U:H5'   | 2.12                     | 0.49              |
| 35:DA:1542:A:C8   | 35:DA:1542:A:H3'   | 2.47                     | 0.49              |
| 35:DA:1899:G:O2'  | 35:DA:1900:A:H5''  | 2.12                     | 0.49              |
| 35:DA:2543:G:H5'  | 35:DA:2543:G:H8    | 1.77                     | 0.49              |
| 35:DA:667:U:H2'   | 35:DA:668:G:O4'    | 2.12                     | 0.49              |
| 35:DA:917:A:H2'   | 35:DA:918:A:O4'    | 2.12                     | 0.49              |
| 36:DB:20:C:C2'    | 36:DB:21:G:H5''    | 2.42                     | 0.49              |
| 36:DB:87:G:H2'    | 36:DB:88:C:H5''    | 1.94                     | 0.49              |
| 37:DC:79:ALA:O    | 37:DC:120:VAL:HG11 | 2.12                     | 0.49              |
| 37:DC:84:ILE:HG12 | 37:DC:96:GLY:O     | 2.11                     | 0.49              |
| 38:DD:77:ALA:HB2  | 38:DD:97:TYR:HA    | 1.93                     | 0.49              |
| 39:DE:69:LYS:O    | 39:DE:70:ALA:C     | 2.49                     | 0.49              |
| 40:DF:192:LEU:CD2 | 40:DF:194:MET:HG3  | 2.26                     | 0.49              |
| 42:DH:103:LEU:HB2 | 42:DH:123:PHE:HD2  | 1.77                     | 0.49              |
| 42:DH:173:PRO:C   | 42:DH:175:LYS:N    | 2.65                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:DH:46:GLU:HG3   | 42:DH:51:ARG:H     | 1.77                     | 0.49              |
| 44:DK:13:PRO:HA    | 44:DK:52:ILE:HA    | 1.94                     | 0.49              |
| 48:DP:140:ALA:O    | 48:DP:141:ALA:HB3  | 2.12                     | 0.49              |
| 48:DP:16:ARG:CZ    | 48:DP:18:ARG:HB2   | 2.42                     | 0.49              |
| 50:DR:48:VAL:O     | 50:DR:49:ASP:C     | 2.50                     | 0.49              |
| 55:DW:59:VAL:HG21  | 55:DW:66:GLU:HB2   | 1.93                     | 0.49              |
| 58:DZ:102:LEU:HD11 | 58:DZ:124:ILE:CG2  | 2.41                     | 0.49              |
| 1:AA:1388:C:H2'    | 1:AA:1389:C:H6     | 1.77                     | 0.49              |
| 1:AA:254:G:HO2'    | 1:AA:255:G:H5'     | 1.77                     | 0.49              |
| 2:AB:137:ARG:HG2   | 2:AB:137:ARG:HH11  | 1.77                     | 0.49              |
| 2:AB:204:ASN:ND2   | 2:AB:204:ASN:C     | 2.65                     | 0.49              |
| 3:AC:51:GLY:O      | 3:AC:115:LEU:HD21  | 2.11                     | 0.49              |
| 4:AD:58:LEU:HD23   | 4:AD:58:LEU:O      | 2.12                     | 0.49              |
| 6:AF:22:GLU:HA     | 6:AF:22:GLU:OE2    | 2.12                     | 0.49              |
| 7:AG:29:LYS:CB     | 7:AG:105:VAL:HG21  | 2.42                     | 0.49              |
| 9:AI:11:LYS:HG2    | 9:AI:11:LYS:O      | 2.11                     | 0.49              |
| 10:AJ:27:ALA:HB2   | 10:AJ:85:LEU:HD11  | 1.92                     | 0.49              |
| 14:AN:41:ARG:HG2   | 14:AN:41:ARG:NH1   | 2.19                     | 0.49              |
| 24:AY:121:VAL:CA   | 24:AY:124:GLN:HE22 | 2.25                     | 0.49              |
| 24:AY:616:TYR:CE2  | 24:AY:664:GLN:HG3  | 2.47                     | 0.49              |
| 35:BA:1666:G:C2'   | 35:BA:1667:G:H5'   | 2.41                     | 0.49              |
| 35:BA:2030:A:H4'   | 35:BA:2031:A:H8    | 1.77                     | 0.49              |
| 35:BA:2051:A:H2'   | 35:BA:2578:G:O5'   | 2.12                     | 0.49              |
| 35:BA:2056:G:N2    | 35:BA:2057:A:N9    | 2.60                     | 0.49              |
| 35:BA:350:U:H2'    | 35:BA:351:G:O4'    | 2.12                     | 0.49              |
| 35:BA:654(P):C:H2' | 35:BA:654(Q):C:O4' | 2.12                     | 0.49              |
| 35:BA:948:G:H1     | 35:BA:969:U:H3     | 1.60                     | 0.49              |
| 36:BB:20:C:C2'     | 36:BB:21:G:H5''    | 2.41                     | 0.49              |
| 36:BB:85:G:O2'     | 36:BB:86:G:H5'     | 2.11                     | 0.49              |
| 36:BB:87:G:H2'     | 36:BB:88:C:H5''    | 1.94                     | 0.49              |
| 37:BC:153:ILE:O    | 37:BC:157:ILE:HG13 | 2.12                     | 0.49              |
| 37:BC:185:LYS:O    | 37:BC:186:LEU:C    | 2.50                     | 0.49              |
| 38:BD:35:LYS:NZ    | 38:BD:35:LYS:HB3   | 2.27                     | 0.49              |
| 39:BE:34:VAL:O     | 39:BE:34:VAL:HG22  | 2.11                     | 0.49              |
| 42:BH:40:GLU:HG3   | 42:BH:64:LEU:HD13  | 1.94                     | 0.49              |
| 43:BJ:69:UNK:O     | 43:BJ:71:UNK:N     | 2.45                     | 0.49              |
| 46:BN:125:GLY:HA3  | 46:BN:126:PRO:C    | 2.32                     | 0.49              |
| 46:BN:132:ALA:O    | 46:BN:133:GLN:CB   | 2.60                     | 0.49              |
| 30:B5:55:ARG:NH1   | 50:BR:33:ARG:HD2   | 2.26                     | 0.49              |
| 51:BS:35:ILE:CD1   | 51:BS:99:LYS:HE3   | 2.42                     | 0.49              |
| 57:BY:12:THR:HG23  | 57:BY:25:GLY:O     | 2.12                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 57:BY:52:SER:N     | 57:BY:53:PRO:CD     | 2.75                     | 0.49              |
| 57:BY:76:CYS:SG    | 57:BY:77:PRO:CD     | 2.86                     | 0.49              |
| 58:BZ:151:HIS:HA   | 58:BZ:171:ILE:CG2   | 2.26                     | 0.49              |
| 1:CA:1081:G:O2'    | 1:CA:1082:G:H5'     | 2.12                     | 0.49              |
| 1:CA:159:G:H2'     | 1:CA:160:A:H5''     | 1.93                     | 0.49              |
| 1:CA:665:A:H2'     | 1:CA:725:G:N2       | 2.27                     | 0.49              |
| 2:CB:17:PHE:CD2    | 2:CB:18:GLY:N       | 2.80                     | 0.49              |
| 4:CD:158:ILE:CG2   | 4:CD:162:LEU:HD12   | 2.43                     | 0.49              |
| 8:CH:17:THR:CG2    | 8:CH:63:LEU:HD12    | 2.42                     | 0.49              |
| 12:CL:70:ILE:HD12  | 12:CL:75:HIS:NE2    | 2.27                     | 0.49              |
| 12:CL:75:HIS:CD2   | 12:CL:77:LEU:HD12   | 2.43                     | 0.49              |
| 14:CN:41:ARG:NH1   | 14:CN:41:ARG:HG2    | 2.24                     | 0.49              |
| 19:CS:72:GLY:C     | 19:CS:74:PHE:H      | 2.15                     | 0.49              |
| 20:CT:23:ARG:HA    | 20:CT:26:ASN:HD21   | 1.77                     | 0.49              |
| 24:CY:329:ARG:HG2  | 24:CY:331:TYR:OH    | 2.12                     | 0.49              |
| 24:CY:528:ALA:O    | 24:CY:568:TYR:HA    | 2.12                     | 0.49              |
| 24:CY:601:ILE:O    | 24:CY:678:GLU:HA    | 2.12                     | 0.49              |
| 25:D0:70:GLN:NE2   | 25:D0:80:HIS:NE2    | 2.60                     | 0.49              |
| 30:D5:36:CYS:O     | 30:D5:36:CYS:SG     | 2.69                     | 0.49              |
| 32:D7:27:GLY:HA2   | 32:D7:30:VAL:HG23   | 1.94                     | 0.49              |
| 31:D6:10:LEU:HB3   | 33:D8:34:TRP:CD1    | 2.47                     | 0.49              |
| 35:DA:2115:G:H3'   | 35:DA:2116:G:C5'    | 2.42                     | 0.49              |
| 35:DA:2206:G:N3    | 35:DA:2206:G:H3'    | 2.27                     | 0.49              |
| 35:DA:2313:C:H5'   | 35:DA:2313:C:C6     | 2.39                     | 0.49              |
| 35:DA:2712:U:C2'   | 35:DA:2712(A):A:O5' | 2.60                     | 0.49              |
| 35:DA:528:A:C2     | 35:DA:2043:C:H5'    | 2.47                     | 0.49              |
| 35:DA:52:A:C2'     | 35:DA:53:A:H5'      | 2.42                     | 0.49              |
| 37:DC:185:LYS:O    | 37:DC:186:LEU:C     | 2.50                     | 0.49              |
| 38:DD:62:TYR:CE1   | 38:DD:64:ILE:HA     | 2.47                     | 0.49              |
| 39:DE:116:VAL:HG22 | 39:DE:122:PHE:CG    | 2.47                     | 0.49              |
| 40:DF:204:ASN:C    | 40:DF:206:ILE:H     | 2.16                     | 0.49              |
| 41:DG:125:PHE:CZ   | 41:DG:170:ARG:HA    | 2.47                     | 0.49              |
| 42:DH:118:PRO:CG   | 42:DH:121:ILE:HD12  | 2.38                     | 0.49              |
| 44:DK:100:THR:OG1  | 44:DK:103:GLN:HG3   | 2.11                     | 0.49              |
| 47:DO:63:VAL:HG23  | 47:DO:64:ARG:HG3    | 1.93                     | 0.49              |
| 52:DT:1:MET:H2     | 52:DT:7:ILE:HD11    | 1.76                     | 0.49              |
| 54:DV:5:VAL:HG23   | 54:DV:37:VAL:O      | 2.11                     | 0.49              |
| 54:DV:99:ILE:H     | 54:DV:99:ILE:HD13   | 1.77                     | 0.49              |
| 55:DW:40:ASN:O     | 55:DW:41:LYS:HG2    | 2.12                     | 0.49              |
| 55:DW:88:ARG:CB    | 55:DW:92:ARG:HB3    | 2.42                     | 0.49              |
| 56:DX:14:SER:H     | 56:DX:17:ALA:HB3    | 1.76                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 58:DZ:43:GLU:O    | 58:DZ:47:VAL:N     | 2.45                     | 0.49              |
| 58:DZ:63:ASP:C    | 58:DZ:65:GLN:H     | 2.16                     | 0.49              |
| 1:AA:1094:G:O2'   | 1:AA:1095:U:OP2    | 2.28                     | 0.49              |
| 1:AA:1144:G:N2    | 1:AA:1146:A:H62    | 2.10                     | 0.49              |
| 1:AA:636:U:H2'    | 1:AA:637:G:C8      | 2.47                     | 0.49              |
| 1:AA:719:C:C2     | 18:AR:50:ILE:HG12  | 2.47                     | 0.49              |
| 2:AB:163:PHE:CD2  | 2:AB:185:ILE:HG13  | 2.47                     | 0.49              |
| 2:AB:215:LEU:O    | 2:AB:218:ALA:HB3   | 2.12                     | 0.49              |
| 3:AC:179:ARG:NH2  | 3:AC:206:GLU:OE2   | 2.45                     | 0.49              |
| 3:AC:54:ARG:HG2   | 3:AC:54:ARG:HH11   | 1.77                     | 0.49              |
| 1:AA:972:C:H4'    | 10:AJ:57:LYS:CB    | 2.42                     | 0.49              |
| 10:AJ:69:ASN:O    | 10:AJ:70:ARG:HG3   | 2.12                     | 0.49              |
| 16:AP:9:PHE:HE2   | 16:AP:18:ARG:HD2   | 1.76                     | 0.49              |
| 18:AR:87:ARG:NH1  | 18:AR:87:ARG:CB    | 2.74                     | 0.49              |
| 22:AW:5:G:C6      | 22:AW:70:C:N4      | 2.77                     | 0.49              |
| 24:AY:210:ARG:O   | 24:AY:214:GLU:HG2  | 2.12                     | 0.49              |
| 24:AY:681:LYS:HD2 | 24:AY:682:GLN:N    | 2.27                     | 0.49              |
| 27:B2:18:PRO:O    | 27:B2:19:VAL:C     | 2.50                     | 0.49              |
| 27:B2:61:LEU:HA   | 27:B2:64:LEU:HB3   | 1.94                     | 0.49              |
| 35:BA:86:C:H4'    | 35:BA:104:U:H1'    | 1.93                     | 0.49              |
| 35:BA:123:G:O2'   | 35:BA:124:G:H5'    | 2.12                     | 0.49              |
| 35:BA:1248:G:N3   | 53:BU:3:ARG:HD2    | 2.26                     | 0.49              |
| 35:BA:1750:G:O2'  | 35:BA:1751:C:H5'   | 2.11                     | 0.49              |
| 35:BA:753:C:H2'   | 35:BA:754:C:H6     | 1.77                     | 0.49              |
| 35:BA:811:U:H3'   | 35:BA:812:C:C5'    | 2.42                     | 0.49              |
| 37:BC:120:VAL:O   | 37:BC:124:VAL:HG23 | 2.12                     | 0.49              |
| 37:BC:34:ALA:CB   | 37:BC:179:ALA:HB2  | 2.43                     | 0.49              |
| 37:BC:34:ALA:HA   | 37:BC:40:GLU:OE2   | 2.12                     | 0.49              |
| 38:BD:48:ARG:HH11 | 38:BD:48:ARG:HG3   | 1.76                     | 0.49              |
| 41:BG:5:VAL:O     | 41:BG:6:ALA:C      | 2.49                     | 0.49              |
| 41:BG:7:LEU:HB3   | 41:BG:100:TRP:HE3  | 1.76                     | 0.49              |
| 45:BL:70:UNK:HA   | 45:BL:73:UNK:CB    | 2.43                     | 0.49              |
| 46:BN:65:LYS:NZ   | 46:BN:65:LYS:CB    | 2.76                     | 0.49              |
| 50:BR:53:HIS:O    | 50:BR:53:HIS:ND1   | 2.43                     | 0.49              |
| 51:BS:74:ALA:HB3  | 51:BS:103:GLU:HG3  | 1.95                     | 0.49              |
| 51:BS:49:VAL:HG22 | 51:BS:80:LEU:HD12  | 1.95                     | 0.49              |
| 53:BU:47:TYR:CA   | 53:BU:50:ARG:NH2   | 2.74                     | 0.49              |
| 57:BY:84:ARG:HB2  | 57:BY:97:ARG:HB2   | 1.92                     | 0.49              |
| 58:BZ:79:ARG:HG3  | 58:BZ:79:ARG:O     | 2.12                     | 0.49              |
| 1:CA:1466:C:H2'   | 1:CA:1467:G:O4'    | 2.12                     | 0.49              |
| 1:CA:1404:C:H1'   | 1:CA:1499:A:N1     | 2.26                     | 0.49              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:177:C:C2      | 1:CA:178:C:C5      | 3.00                     | 0.49              |
| 1:CA:509:A:H2      | 1:CA:543:C:H1'     | 1.76                     | 0.49              |
| 4:CD:57:ARG:NH1    | 4:CD:205:GLU:OE2   | 2.45                     | 0.49              |
| 17:CQ:67:LYS:O     | 17:CQ:69:LYS:N     | 2.44                     | 0.49              |
| 22:CV:76:A:H4'     | 22:CV:76:A:OP1     | 2.12                     | 0.49              |
| 24:CY:227:ILE:HG23 | 24:CY:237:PRO:CG   | 2.37                     | 0.49              |
| 24:CY:32:ILE:HG23  | 24:CY:273:LEU:HD21 | 1.94                     | 0.49              |
| 24:CY:336:THR:HG22 | 24:CY:337:SER:N    | 2.27                     | 0.49              |
| 24:CY:506:GLN:HA   | 24:CY:506:GLN:OE1  | 2.11                     | 0.49              |
| 24:CY:510:VAL:HA   | 24:CY:570:GLY:HA3  | 1.94                     | 0.49              |
| 26:D1:90:ILE:HG22  | 26:D1:94:LEU:CD1   | 2.42                     | 0.49              |
| 31:D6:15:GLU:O     | 31:D6:16:CYS:O     | 2.30                     | 0.49              |
| 31:D6:54:ILE:HD13  | 35:DA:2420:C:C5'   | 2.42                     | 0.49              |
| 35:DA:1556:C:H2'   | 35:DA:1557:C:C6    | 2.47                     | 0.49              |
| 35:DA:1827:C:H2'   | 35:DA:1828:G:O4'   | 2.12                     | 0.49              |
| 35:DA:2308:G:N2    | 41:DG:79:ASN:CB    | 2.74                     | 0.49              |
| 35:DA:2454:G:H2'   | 35:DA:2455:G:H5'   | 1.94                     | 0.49              |
| 38:DD:26:LYS:O     | 38:DD:27:THR:CB    | 2.61                     | 0.49              |
| 39:DE:59:VAL:HG21  | 39:DE:63:LEU:HA    | 1.93                     | 0.49              |
| 40:DF:168:ARG:HG3  | 40:DF:175:THR:HB   | 1.93                     | 0.49              |
| 41:DG:129:GLY:O    | 41:DG:130:ASN:CG   | 2.51                     | 0.49              |
| 41:DG:39:ILE:CG1   | 41:DG:92:VAL:HG23  | 2.42                     | 0.49              |
| 41:DG:57:ALA:O     | 41:DG:60:LEU:HB3   | 2.11                     | 0.49              |
| 48:DP:144:GLU:HG2  | 48:DP:144:GLU:O    | 2.12                     | 0.49              |
| 50:DR:18:LEU:HD23  | 50:DR:19:ALA:N     | 2.27                     | 0.49              |
| 51:DS:85:VAL:O     | 51:DS:106:ARG:HG2  | 2.13                     | 0.49              |
| 52:DT:66:VAL:HA    | 52:DT:71:GLY:HA2   | 1.94                     | 0.49              |
| 35:DA:2019:A:O3'   | 53:DU:27:LEU:HD12  | 2.12                     | 0.49              |
| 57:DY:47:LYS:O     | 57:DY:48:ALA:O     | 2.30                     | 0.49              |
| 44:DK:93:ARG:HB2   | 58:DZ:112:ARG:HH21 | 1.76                     | 0.49              |
| 1:AA:1133:G:C4     | 1:AA:1142:G:N2     | 2.80                     | 0.49              |
| 1:AA:159:G:C2'     | 1:AA:160:A:H5''    | 2.42                     | 0.49              |
| 1:AA:189(D):C:H2'  | 1:AA:189(E):U:O4'  | 2.11                     | 0.49              |
| 1:AA:308:C:H2'     | 1:AA:309:G:H8      | 1.78                     | 0.49              |
| 1:AA:719:C:O2'     | 18:AR:49:LYS:HB3   | 2.12                     | 0.49              |
| 3:AC:140:ARG:HH11  | 3:AC:140:ARG:HG3   | 1.76                     | 0.49              |
| 4:AD:8:VAL:C       | 4:AD:10:ARG:H      | 2.14                     | 0.49              |
| 5:AE:127:ASN:O     | 5:AE:131:ILE:HG12  | 2.12                     | 0.49              |
| 5:AE:28:PHE:CD2    | 5:AE:51:VAL:HG22   | 2.48                     | 0.49              |
| 7:AG:82:GLY:HA3    | 23:AX:13:A:C2      | 2.47                     | 0.49              |
| 8:AH:104:ARG:O     | 8:AH:107:LEU:N     | 2.46                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:AO:33:THR:HG23  | 15:AO:63:ARG:HH12  | 1.78                     | 0.49              |
| 16:AP:7:ALA:O      | 16:AP:17:TYR:HA    | 2.11                     | 0.49              |
| 24:AY:16:GLY:N     | 24:AY:101:LEU:HD13 | 2.27                     | 0.49              |
| 24:AY:125:ALA:C    | 24:AY:127:LYS:N    | 2.66                     | 0.49              |
| 24:AY:340:TYR:CE2  | 24:AY:351:ARG:HD3  | 2.47                     | 0.49              |
| 24:AY:8:ASP:O      | 24:AY:10:LYS:N     | 2.44                     | 0.49              |
| 25:B0:45:PHE:O     | 25:B0:59:LEU:HD11  | 2.12                     | 0.49              |
| 30:B5:4:HIS:CB     | 30:B5:5:PRO:CD     | 2.89                     | 0.49              |
| 35:BA:1248:G:C4    | 53:BU:3:ARG:HD2    | 2.47                     | 0.49              |
| 35:BA:1536:C:H2'   | 35:BA:1537:G:H4'   | 1.94                     | 0.49              |
| 35:BA:1719:G:C2'   | 35:BA:1720:U:H5'   | 2.41                     | 0.49              |
| 35:BA:2050:C:H1'   | 39:BE:156:MET:CE   | 2.43                     | 0.49              |
| 35:BA:2470:G:P     | 49:BQ:56:ARG:NH1   | 2.82                     | 0.49              |
| 35:BA:1669:A:H4'   | 35:BA:2549:G:H4'   | 1.94                     | 0.49              |
| 35:BA:2787:C:O2    | 39:BE:61:ARG:HD3   | 2.12                     | 0.49              |
| 35:BA:363(A):A:H2' | 35:BA:363(B):G:C8  | 2.46                     | 0.49              |
| 35:BA:614(A):U:O2' | 35:BA:614(B):G:H5' | 2.12                     | 0.49              |
| 35:BA:796:C:H2'    | 35:BA:797:C:H6     | 1.75                     | 0.49              |
| 35:BA:876:C:H2'    | 35:BA:877:U:O4'    | 2.12                     | 0.49              |
| 37:BC:30:VAL:O     | 37:BC:33:LEU:N     | 2.45                     | 0.49              |
| 38:BD:213:ARG:C    | 38:BD:215:LEU:H    | 2.16                     | 0.49              |
| 39:BE:69:LYS:O     | 39:BE:71:GLY:N     | 2.45                     | 0.49              |
| 35:BA:2653:U:O2'   | 42:BH:110:SER:HB3  | 2.12                     | 0.49              |
| 44:BK:41:PHE:C     | 44:BK:43:ALA:H     | 2.16                     | 0.49              |
| 48:BP:147:LEU:O    | 48:BP:148:LEU:HB2  | 2.12                     | 0.49              |
| 52:BT:82:LEU:HD23  | 52:BT:85:LYS:HD2   | 1.92                     | 0.49              |
| 46:BN:2:LYS:NZ     | 54:BV:12:TYR:HA    | 2.27                     | 0.49              |
| 56:BX:34:ALA:HA    | 56:BX:38:GLU:OE2   | 2.13                     | 0.49              |
| 1:CA:1225:A:H3'    | 1:CA:1226:C:C6     | 2.47                     | 0.49              |
| 1:CA:174:C:H2'     | 1:CA:175:C:H6      | 1.77                     | 0.49              |
| 1:CA:460:G:O6      | 1:CA:470:C:H4'     | 2.11                     | 0.49              |
| 1:CA:936:C:H2'     | 1:CA:937:A:O4'     | 2.12                     | 0.49              |
| 2:CB:82:ARG:HH11   | 2:CB:82:ARG:HG3    | 1.77                     | 0.49              |
| 3:CC:123:GLN:HB3   | 3:CC:128:PHE:CD2   | 2.45                     | 0.49              |
| 3:CC:35:GLU:O      | 3:CC:39:ILE:HG13   | 2.12                     | 0.49              |
| 4:CD:199:ASN:OD1   | 4:CD:201:GLN:HB2   | 2.13                     | 0.49              |
| 4:CD:62:GLN:O      | 4:CD:66:ARG:HB2    | 2.12                     | 0.49              |
| 13:CM:91:ARG:HH21  | 19:CS:81:ARG:NH2   | 2.10                     | 0.49              |
| 15:CO:31:LEU:N     | 15:CO:31:LEU:CD2   | 2.76                     | 0.49              |
| 15:CO:50:HIS:O     | 15:CO:53:HIS:HB3   | 2.12                     | 0.49              |
| 18:CR:87:ARG:NH1   | 18:CR:87:ARG:CB    | 2.76                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:CS:62:ILE:O     | 19:CS:62:ILE:HG13  | 2.12                     | 0.49              |
| 21:CU:10:ARG:O     | 21:CU:13:ILE:N     | 2.45                     | 0.49              |
| 22:CV:59:A:C2'     | 22:CV:60:U:H5'     | 2.41                     | 0.49              |
| 24:CY:439:ARG:HB2  | 24:CY:452:SER:CB   | 2.43                     | 0.49              |
| 24:CY:491:VAL:HG21 | 24:CY:597:GLY:CA   | 2.42                     | 0.49              |
| 24:CY:138:LYS:HE2  | 62:CY:703:GDP:N9   | 2.27                     | 0.49              |
| 25:D0:20:ARG:HG2   | 25:D0:20:ARG:HH11  | 1.77                     | 0.49              |
| 22:CV:2:G:H5'      | 25:D0:8:GLY:HA2    | 1.95                     | 0.49              |
| 26:D1:61:ARG:HH11  | 26:D1:61:ARG:CB    | 2.23                     | 0.49              |
| 27:D2:65:ASN:HD21  | 35:DA:112:U:H5'    | 1.76                     | 0.49              |
| 35:DA:1368:G:O2'   | 35:DA:1369:G:H5'   | 2.13                     | 0.49              |
| 35:DA:2075:U:C2'   | 35:DA:2076:U:H5''  | 2.42                     | 0.49              |
| 33:D8:31:HIS:HE1   | 35:DA:2392:A:OP2   | 1.94                     | 0.49              |
| 35:DA:244:A:H1'    | 35:DA:255:A:N6     | 2.28                     | 0.49              |
| 35:DA:2564:A:OP1   | 35:DA:2648:C:H4'   | 2.12                     | 0.49              |
| 35:DA:2653:U:O2'   | 42:DH:110:SER:HB3  | 2.12                     | 0.49              |
| 35:DA:478:A:C6     | 35:DA:480:A:C6     | 3.01                     | 0.49              |
| 35:DA:515:A:C2     | 35:DA:1261:C:H1'   | 2.48                     | 0.49              |
| 35:DA:545:C:H2'    | 35:DA:547:A:C5'    | 2.32                     | 0.49              |
| 35:DA:650:C:C2'    | 35:DA:651:G:H5''   | 2.42                     | 0.49              |
| 35:DA:654(O):G:H2' | 35:DA:654(P):C:C6  | 2.48                     | 0.49              |
| 35:DA:769:G:H4'    | 35:DA:1379:A:N1    | 2.27                     | 0.49              |
| 35:DA:769:G:H2'    | 35:DA:770:G:H8     | 1.77                     | 0.49              |
| 38:DD:108:PRO:HG2  | 38:DD:111:LEU:HB2  | 1.93                     | 0.49              |
| 38:DD:142:VAL:HG23 | 38:DD:193:VAL:HA   | 1.95                     | 0.49              |
| 39:DE:119:ARG:HD2  | 39:DE:120:TRP:NE1  | 2.27                     | 0.49              |
| 42:DH:104:GLU:HA   | 42:DH:113:VAL:O    | 2.11                     | 0.49              |
| 42:DH:68:THR:C     | 42:DH:70:THR:H     | 2.15                     | 0.49              |
| 44:DK:41:PHE:C     | 44:DK:43:ALA:H     | 2.16                     | 0.49              |
| 45:DL:64:UNK:O     | 45:DL:65:UNK:C     | 2.59                     | 0.49              |
| 46:DN:120:LEU:CD1  | 46:DN:122:VAL:HG23 | 2.41                     | 0.49              |
| 48:DP:108:LYS:C    | 48:DP:110:TYR:N    | 2.65                     | 0.49              |
| 35:DA:2875:C:O2'   | 52:DT:5:ALA:HB3    | 2.12                     | 0.49              |
| 53:DU:92:ARG:CD    | 53:DU:94:ASN:HB3   | 2.41                     | 0.49              |
| 57:DY:84:ARG:HB2   | 57:DY:97:ARG:HB2   | 1.94                     | 0.49              |
| 58:DZ:127:LYS:HB3  | 58:DZ:127:LYS:NZ   | 2.26                     | 0.49              |
| 1:AA:1216:G:OP1    | 14:AN:2:ALA:HA     | 2.13                     | 0.49              |
| 1:AA:392:G:H2'     | 1:AA:393:A:H8      | 1.77                     | 0.49              |
| 1:AA:392:G:H2'     | 1:AA:393:A:C8      | 2.48                     | 0.49              |
| 1:AA:678:U:H2'     | 1:AA:679:C:C6      | 2.47                     | 0.49              |
| 6:AF:29:ALA:O      | 6:AF:31:GLU:N      | 2.45                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:AL:26:ALA:O     | 12:AL:27:LEU:O     | 2.31                     | 0.49              |
| 19:AS:72:GLY:C     | 19:AS:74:PHE:H     | 2.14                     | 0.49              |
| 24:AY:122:TRP:CZ3  | 24:AY:132:ARG:HD2  | 2.48                     | 0.49              |
| 24:AY:181:LEU:HD23 | 24:AY:182:ARG:HH12 | 1.77                     | 0.49              |
| 24:AY:18:ALA:O     | 24:AY:19:ALA:CB    | 2.59                     | 0.49              |
| 24:AY:21:ILE:H     | 24:AY:21:ILE:CD1   | 2.20                     | 0.49              |
| 24:AY:252:ASP:O    | 24:AY:253:LEU:HB2  | 2.12                     | 0.49              |
| 24:AY:298:VAL:HG13 | 24:AY:299:VAL:N    | 2.26                     | 0.49              |
| 24:AY:510:VAL:CG1  | 24:AY:567:LEU:HD13 | 2.42                     | 0.49              |
| 25:B0:23:VAL:HG11  | 25:B0:69:PHE:HZ    | 1.77                     | 0.49              |
| 26:B1:76:ARG:HH12  | 26:B1:95:LEU:CD2   | 2.15                     | 0.49              |
| 26:B1:76:ARG:HH22  | 26:B1:95:LEU:CB    | 2.24                     | 0.49              |
| 27:B2:13:ALA:C     | 27:B2:15:LYS:H     | 2.16                     | 0.49              |
| 28:B3:38:GLU:HB3   | 28:B3:43:ILE:HG13  | 1.93                     | 0.49              |
| 30:B5:40:LYS:HE2   | 30:B5:46:CYS:CB    | 2.42                     | 0.49              |
| 31:B6:10:LEU:N     | 31:B6:10:LEU:HD23  | 2.27                     | 0.49              |
| 33:B8:4:MET:CE     | 33:B8:61:LEU:HD22  | 2.42                     | 0.49              |
| 33:B8:62:LEU:N     | 33:B8:63:PRO:CD    | 2.75                     | 0.49              |
| 34:B9:27:CYS:SG    | 34:B9:29:ASN:ND2   | 2.84                     | 0.49              |
| 35:BA:1722:A:H2    | 35:BA:1740:G:H2'   | 1.76                     | 0.49              |
| 35:BA:1858:G:O2'   | 35:BA:1884:A:N6    | 2.45                     | 0.49              |
| 35:BA:552:G:O2'    | 35:BA:553:G:H5'    | 2.12                     | 0.49              |
| 38:BD:24:ILE:CG1   | 38:BD:25:THR:N     | 2.74                     | 0.49              |
| 38:BD:183:ARG:HD2  | 38:BD:270:ILE:HG23 | 1.94                     | 0.49              |
| 39:BE:57:LYS:HZ3   | 39:BE:63:LEU:HG    | 1.77                     | 0.49              |
| 40:BF:107:LYS:O    | 40:BF:108:LYS:C    | 2.50                     | 0.49              |
| 40:BF:10:PRO:HG2   | 40:BF:11:VAL:H     | 1.77                     | 0.49              |
| 40:BF:9:ILE:HG12   | 40:BF:14:PRO:HA    | 1.93                     | 0.49              |
| 40:BF:179:GLU:C    | 40:BF:181:LEU:H    | 2.16                     | 0.49              |
| 41:BG:77:ILE:CG2   | 41:BG:80:PHE:HB2   | 2.42                     | 0.49              |
| 42:BH:33:LEU:HD12  | 42:BH:75:ALA:O     | 2.13                     | 0.49              |
| 42:BH:34:GLU:O     | 42:BH:36:PRO:HD3   | 2.11                     | 0.49              |
| 35:BA:1035:U:O5'   | 42:BH:59:ARG:NH1   | 2.46                     | 0.49              |
| 42:BH:40:GLU:HG3   | 42:BH:64:LEU:CD1   | 2.43                     | 0.49              |
| 44:BK:120:LEU:HA   | 44:BK:123:ALA:HB3  | 1.95                     | 0.49              |
| 49:BQ:1:MET:HE1    | 49:BQ:45:GLN:N     | 2.27                     | 0.49              |
| 52:BT:106:SER:C    | 52:BT:107:ASP:OD1  | 2.51                     | 0.49              |
| 52:BT:91:ARG:O     | 52:BT:117:ASP:CB   | 2.61                     | 0.49              |
| 52:BT:10:VAL:O     | 52:BT:11:GLU:C     | 2.51                     | 0.49              |
| 53:BU:70:ARG:NH2   | 53:BU:75:ASN:HB2   | 2.27                     | 0.49              |
| 56:BX:68:ARG:O     | 56:BX:68:ARG:HD3   | 2.12                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:BY:47:LYS:HG3   | 57:BY:60:PHE:CE2   | 2.42                     | 0.49              |
| 1:CA:1399:C:C2     | 1:CA:1502:A:N6     | 2.80                     | 0.49              |
| 1:CA:15:G:H4'      | 5:CE:24:ARG:NH1    | 2.27                     | 0.49              |
| 1:CA:559:A:P       | 5:CE:126:ARG:HH22  | 2.35                     | 0.49              |
| 1:CA:948:C:H2'     | 1:CA:949:A:H8      | 1.77                     | 0.49              |
| 2:CB:223:ILE:O     | 2:CB:226:ARG:N     | 2.45                     | 0.49              |
| 3:CC:46:GLU:O      | 3:CC:47:LEU:CB     | 2.55                     | 0.49              |
| 1:CA:619:U:N3      | 4:CD:134:ASP:OD2   | 2.39                     | 0.49              |
| 18:CR:31:LEU:HD23  | 18:CR:31:LEU:N     | 2.24                     | 0.49              |
| 1:CA:323:U:H5'     | 20:CT:23:ARG:HB2   | 1.95                     | 0.49              |
| 22:CW:37:U:H2'     | 22:CW:38:A:C8      | 2.47                     | 0.49              |
| 24:CY:182:ARG:HG2  | 24:CY:239:GLU:OE2  | 2.12                     | 0.49              |
| 24:CY:250:THR:HA   | 24:CY:255:ILE:HG23 | 1.95                     | 0.49              |
| 24:CY:440:VAL:HG12 | 24:CY:449:THR:CG2  | 2.42                     | 0.49              |
| 24:CY:533:VAL:HB   | 24:CY:570:GLY:O    | 2.12                     | 0.49              |
| 24:CY:630:GLN:NE2  | 24:CY:646:PHE:HB2  | 2.28                     | 0.49              |
| 25:D0:12:ASN:O     | 25:D0:14:ARG:N     | 2.41                     | 0.49              |
| 29:D4:48:ARG:HG2   | 29:D4:48:ARG:O     | 2.11                     | 0.49              |
| 30:D5:40:LYS:HE2   | 30:D5:46:CYS:CB    | 2.42                     | 0.49              |
| 33:D8:62:LEU:N     | 33:D8:63:PRO:CD    | 2.76                     | 0.49              |
| 34:D9:26:ILE:HG22  | 34:D9:27:CYS:N     | 2.27                     | 0.49              |
| 35:DA:1028:A:H61   | 35:DA:1125:G:H2'   | 1.75                     | 0.49              |
| 35:DA:1132:A:H2'   | 35:DA:1133:U:H6    | 1.77                     | 0.49              |
| 35:DA:154(A):C:C5  | 35:DA:155:U:H1'    | 2.47                     | 0.49              |
| 35:DA:1750:G:O2'   | 35:DA:1751:C:H5'   | 2.13                     | 0.49              |
| 35:DA:644:A:C2     | 35:DA:2369:A:H1'   | 2.47                     | 0.49              |
| 35:DA:2481:G:O2'   | 35:DA:2482:G:P     | 2.70                     | 0.49              |
| 35:DA:2872:G:C2    | 35:DA:2873:A:N6    | 2.81                     | 0.49              |
| 35:DA:408:G:O2'    | 35:DA:409:C:H5'    | 2.12                     | 0.49              |
| 35:DA:979:G:H2'    | 35:DA:982:C:N4     | 2.28                     | 0.49              |
| 37:DC:34:ALA:HA    | 37:DC:40:GLU:OE2   | 2.13                     | 0.49              |
| 35:DA:2130:U:OP1   | 37:DC:6:LYS:HB2    | 2.13                     | 0.49              |
| 35:DA:1654:A:C2    | 39:DE:113:PHE:CD1  | 3.01                     | 0.49              |
| 40:DF:185:ASP:HA   | 40:DF:188:ARG:HD3  | 1.94                     | 0.49              |
| 42:DH:121:ILE:HA   | 42:DH:134:SER:O    | 2.13                     | 0.49              |
| 42:DH:50:VAL:HG12  | 42:DH:51:ARG:N     | 2.26                     | 0.49              |
| 42:DH:46:GLU:CD    | 42:DH:51:ARG:HB2   | 2.32                     | 0.49              |
| 35:DA:1996:C:OP1   | 47:DO:31:LYS:HE2   | 2.13                     | 0.49              |
| 48:DP:147:LEU:O    | 48:DP:148:LEU:HB2  | 2.11                     | 0.49              |
| 51:DS:89:ARG:CG    | 51:DS:92:TYR:CA    | 2.87                     | 0.49              |
| 52:DT:102:ILE:HB   | 52:DT:110:ILE:HD12 | 1.94                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:DT:83:ILE:CG1   | 52:DT:84:GLN:N     | 2.74                     | 0.49              |
| 1:AA:297:G:H4'     | 1:AA:557:G:H4'     | 1.95                     | 0.49              |
| 1:AA:995:C:O2'     | 1:AA:996:A:H5'     | 2.13                     | 0.49              |
| 2:AB:149:LEU:O     | 2:AB:150:SER:C     | 2.50                     | 0.49              |
| 2:AB:54:THR:HG21   | 2:AB:201:ILE:HD11  | 1.94                     | 0.49              |
| 4:AD:8:VAL:C       | 4:AD:10:ARG:N      | 2.66                     | 0.49              |
| 10:AJ:33:GLN:H     | 10:AJ:75:ILE:HD11  | 1.77                     | 0.49              |
| 24:AY:168:ILE:HD11 | 24:AY:178:ILE:CD1  | 2.43                     | 0.49              |
| 24:AY:466:LEU:O    | 24:AY:470:PHE:HB2  | 2.12                     | 0.49              |
| 24:AY:539:ILE:HD12 | 24:AY:567:LEU:CD2  | 2.42                     | 0.49              |
| 26:B1:81:LYS:HZ1   | 35:BA:271(I):G:P   | 2.34                     | 0.49              |
| 29:B4:43:TYR:CD2   | 29:B4:44:THR:HG23  | 2.47                     | 0.49              |
| 30:B5:35:GLU:O     | 30:B5:36:CYS:HB3   | 2.12                     | 0.49              |
| 31:B6:33:LYS:HG2   | 31:B6:34:LEU:N     | 2.28                     | 0.49              |
| 35:BA:1081:U:O3'   | 44:BK:117:THR:HG22 | 2.13                     | 0.49              |
| 35:BA:1169:G:N2    | 35:BA:1181:C:N3    | 2.61                     | 0.49              |
| 30:B5:24:ALA:HB2   | 35:BA:15:G:OP1     | 2.12                     | 0.49              |
| 35:BA:1891:G:H2'   | 35:BA:1892:C:O4'   | 2.12                     | 0.49              |
| 35:BA:211:A:C3'    | 35:BA:212:G:H5''   | 2.41                     | 0.49              |
| 31:B6:24:GLU:OE2   | 35:BA:2346:A:H8    | 1.95                     | 0.49              |
| 31:B6:54:ILE:HD13  | 35:BA:2420:C:C5'   | 2.41                     | 0.49              |
| 26:B1:81:LYS:CE    | 35:BA:271(H):G:H4' | 2.33                     | 0.49              |
| 35:BA:585:G:H2'    | 35:BA:1251:C:H42   | 1.77                     | 0.49              |
| 35:BA:680:G:H2'    | 35:BA:681:G:H8     | 1.77                     | 0.49              |
| 35:BA:825:C:C2'    | 35:BA:826:U:H5'    | 2.43                     | 0.49              |
| 36:BB:81:G:H2'     | 36:BB:82:G:H5'     | 1.94                     | 0.49              |
| 39:BE:38:THR:O     | 39:BE:42:ASP:HB2   | 2.12                     | 0.49              |
| 39:BE:93:VAL:C     | 39:BE:95:ILE:H     | 2.15                     | 0.49              |
| 40:BF:156:LEU:HD21 | 40:BF:163:VAL:HG12 | 1.95                     | 0.49              |
| 41:BG:35:GLU:O     | 41:BG:36:LYS:HB3   | 2.10                     | 0.49              |
| 44:BK:17:ALA:HB3   | 44:BK:38:VAL:CG2   | 2.38                     | 0.49              |
| 47:BO:69:ILE:HB    | 47:BO:77:ILE:HG22  | 1.95                     | 0.49              |
| 48:BP:7:ARG:HG3    | 48:BP:7:ARG:HH11   | 1.77                     | 0.49              |
| 50:BR:18:LEU:HD23  | 50:BR:19:ALA:N     | 2.28                     | 0.49              |
| 51:BS:89:ARG:HE    | 51:BS:91:PRO:HG2   | 1.78                     | 0.49              |
| 54:BV:46:VAL:O     | 54:BV:47:VAL:HG13  | 2.13                     | 0.49              |
| 57:BY:46:LYS:HB2   | 57:BY:62:GLU:HB2   | 1.95                     | 0.49              |
| 58:BZ:79:ARG:O     | 58:BZ:80:ARG:CB    | 2.53                     | 0.49              |
| 1:CA:1064:G:H21    | 1:CA:1190:G:H2'    | 1.77                     | 0.49              |
| 1:CA:1348:U:H2'    | 1:CA:1349:A:C8     | 2.45                     | 0.49              |
| 1:CA:1371:G:O3'    | 9:CI:69:GLY:HA3    | 2.12                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:344:A:H5''    | 1:CA:345:C:OP2     | 2.12                     | 0.49              |
| 1:CA:719:C:O2      | 18:CR:50:ILE:HG12  | 2.13                     | 0.49              |
| 1:CA:78:G:H1       | 1:CA:91:C:H42      | 1.59                     | 0.49              |
| 2:CB:101:MET:HG2   | 2:CB:152:PHE:CE2   | 2.48                     | 0.49              |
| 2:CB:149:LEU:O     | 2:CB:150:SER:C     | 2.50                     | 0.49              |
| 2:CB:15:VAL:H      | 2:CB:16:HIS:CE1    | 2.31                     | 0.49              |
| 2:CB:221:LEU:O     | 2:CB:221:LEU:HD13  | 2.12                     | 0.49              |
| 3:CC:126:ARG:HD2   | 3:CC:128:PHE:CZ    | 2.47                     | 0.49              |
| 3:CC:156:ARG:NH2   | 3:CC:160:ALA:O     | 2.45                     | 0.49              |
| 3:CC:43:LEU:HD22   | 3:CC:47:LEU:HD22   | 1.95                     | 0.49              |
| 3:CC:5:ILE:H       | 3:CC:5:ILE:CD1     | 2.26                     | 0.49              |
| 8:CH:35:ILE:HG22   | 8:CH:39:LEU:HD21   | 1.95                     | 0.49              |
| 8:CH:63:LEU:HD22   | 8:CH:63:LEU:N      | 2.26                     | 0.49              |
| 15:CO:31:LEU:HD22  | 15:CO:31:LEU:N     | 2.28                     | 0.49              |
| 15:CO:65:ARG:H     | 15:CO:65:ARG:HD2   | 1.77                     | 0.49              |
| 22:CW:43:G:N2      | 22:CW:44:A:H1'     | 2.27                     | 0.49              |
| 24:CY:34:TYR:CD2   | 24:CY:35:TYR:CE2   | 3.01                     | 0.49              |
| 24:CY:441:SER:C    | 24:CY:449:THR:HG23 | 2.33                     | 0.49              |
| 26:D1:56:GLN:HE22  | 26:D1:87:PRO:CB    | 2.24                     | 0.49              |
| 32:D7:41:ARG:NH2   | 35:DA:460:A:OP1    | 2.46                     | 0.49              |
| 35:DA:1058:G:H21   | 44:DK:126:MET:HE1  | 1.77                     | 0.49              |
| 35:DA:1095:A:H2'   | 35:DA:1096:A:C8    | 2.47                     | 0.49              |
| 35:DA:190:A:H2'    | 35:DA:191:A:C8     | 2.47                     | 0.49              |
| 35:DA:2062:A:O4'   | 35:DA:2062:A:N3    | 2.45                     | 0.49              |
| 35:DA:246:C:C2'    | 35:DA:247:G:H5'    | 2.42                     | 0.49              |
| 35:DA:363(F):A:O2' | 35:DA:364:C:P      | 2.70                     | 0.49              |
| 35:DA:428:A:H3'    | 35:DA:429:A:C8     | 2.47                     | 0.49              |
| 35:DA:876:C:H2'    | 35:DA:877:U:O4'    | 2.13                     | 0.49              |
| 38:DD:11:PRO:C     | 38:DD:13:ARG:N     | 2.66                     | 0.49              |
| 38:DD:213:ARG:C    | 38:DD:215:LEU:H    | 2.15                     | 0.49              |
| 38:DD:73:VAL:O     | 38:DD:75:ILE:HG12  | 2.11                     | 0.49              |
| 39:DE:104:VAL:HG22 | 39:DE:198:VAL:HG22 | 1.92                     | 0.49              |
| 39:DE:55:ASN:C     | 39:DE:57:LYS:H     | 2.16                     | 0.49              |
| 40:DF:176:LEU:HD11 | 40:DF:180:GLY:HA3  | 1.94                     | 0.49              |
| 40:DF:206:ILE:HG22 | 40:DF:207:GLY:H    | 1.78                     | 0.49              |
| 41:DG:77:ILE:O     | 41:DG:78:SER:C     | 2.49                     | 0.49              |
| 42:DH:172:LYS:HB3  | 42:DH:175:LYS:HB3  | 1.94                     | 0.49              |
| 46:DN:132:ALA:O    | 46:DN:133:GLN:HB2  | 2.12                     | 0.49              |
| 35:DA:598:G:C5'    | 48:DP:15:ARG:HB2   | 2.38                     | 0.49              |
| 49:DQ:58:PHE:HD1   | 49:DQ:58:PHE:O     | 1.96                     | 0.49              |
| 50:DR:97:VAL:O     | 50:DR:98:LEU:HD23  | 2.12                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 54:DV:28:GLU:CB    | 54:DV:31:ALA:HB2   | 2.36                     | 0.49              |
| 54:DV:46:VAL:HG13  | 54:DV:47:VAL:N     | 2.27                     | 0.49              |
| 53:DU:112:ARG:CZ   | 54:DV:46:VAL:HG21  | 2.42                     | 0.49              |
| 58:DZ:130:PRO:CA   | 58:DZ:133:ILE:HD11 | 2.38                     | 0.49              |
| 1:AA:1271:G:H2'    | 1:AA:1272:G:H8     | 1.77                     | 0.49              |
| 1:AA:1281:U:H5'    | 1:AA:1282:C:OP2    | 2.13                     | 0.49              |
| 1:AA:190:U:O2'     | 1:AA:191:G:H5'     | 2.12                     | 0.49              |
| 1:AA:560:U:H4'     | 1:AA:561:U:H5''    | 1.94                     | 0.49              |
| 1:AA:686:U:O2'     | 1:AA:687:A:H8      | 1.79                     | 0.49              |
| 2:AB:17:PHE:CD2    | 2:AB:18:GLY:N      | 2.81                     | 0.49              |
| 3:AC:72:LYS:CA     | 3:AC:72:LYS:HE3    | 2.43                     | 0.49              |
| 6:AF:62:TRP:CD1    | 18:AR:35:ARG:NH1   | 2.81                     | 0.49              |
| 12:AL:115:LYS:O    | 12:AL:117:ARG:HG3  | 2.13                     | 0.49              |
| 13:AM:56:LEU:HD13  | 13:AM:60:VAL:HG23  | 1.94                     | 0.49              |
| 15:AO:9:GLN:O      | 15:AO:10:LYS:C     | 2.51                     | 0.49              |
| 18:AR:59:SER:N     | 18:AR:62:GLU:HB2   | 2.24                     | 0.49              |
| 19:AS:79:THR:HG22  | 19:AS:80:TYR:N     | 2.27                     | 0.49              |
| 13:AM:91:ARG:HH21  | 19:AS:81:ARG:NH2   | 2.10                     | 0.49              |
| 24:AY:85:PRO:HG3   | 24:AY:94:VAL:HG13  | 1.95                     | 0.49              |
| 25:B0:10:THR:HG22  | 25:B0:11:ARG:N     | 2.27                     | 0.49              |
| 26:B1:4:VAL:HG21   | 26:B1:11:ARG:NH1   | 2.27                     | 0.49              |
| 26:B1:86:SER:HA    | 26:B1:89:GLU:CD    | 2.33                     | 0.49              |
| 27:B2:50:ILE:C     | 27:B2:52:ASP:N     | 2.65                     | 0.49              |
| 27:B2:7:ARG:HG3    | 27:B2:7:ARG:NH1    | 2.27                     | 0.49              |
| 31:B6:17:LYS:HB2   | 31:B6:44:ARG:NH1   | 2.27                     | 0.49              |
| 35:BA:142(A):C:O2' | 35:BA:1597:A:H5''  | 2.13                     | 0.49              |
| 35:BA:884:C:N4     | 35:BA:886:C:H42    | 2.10                     | 0.49              |
| 35:BA:848:G:C4     | 35:BA:933:A:H8     | 2.31                     | 0.49              |
| 35:BA:991:C:C6     | 35:BA:991:C:H5'    | 2.40                     | 0.49              |
| 38:BD:224:ALA:O    | 38:BD:225:ALA:HB2  | 2.13                     | 0.49              |
| 38:BD:99:ASP:OD2   | 38:BD:99:ASP:C     | 2.51                     | 0.49              |
| 39:BE:176:ILE:CG2  | 39:BE:178:GLU:HB3  | 2.37                     | 0.49              |
| 40:BF:192:LEU:HD23 | 40:BF:193:VAL:N    | 2.26                     | 0.49              |
| 41:BG:102:PHE:O    | 41:BG:104:GLU:N    | 2.46                     | 0.49              |
| 41:BG:29:TRP:C     | 41:BG:31:VAL:N     | 2.64                     | 0.49              |
| 44:BK:39:LYS:O     | 44:BK:43:ALA:HB2   | 2.13                     | 0.49              |
| 47:BO:63:VAL:HG23  | 47:BO:64:ARG:HG3   | 1.94                     | 0.49              |
| 49:BQ:3:MET:HG3    | 49:BQ:4:PRO:O      | 2.12                     | 0.49              |
| 35:BA:1654:A:OP2   | 50:BR:3:HIS:HB2    | 2.12                     | 0.49              |
| 52:BT:102:ILE:O    | 52:BT:106:SER:HB3  | 2.12                     | 0.49              |
| 1:CA:1376:U:H2'    | 1:CA:1377:A:C8     | 2.47                     | 0.49              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:489:C:H2'     | 1:CA:490:G:C8      | 2.48                     | 0.49              |
| 1:CA:490:G:H2'     | 1:CA:491:G:C8      | 2.42                     | 0.49              |
| 1:CA:738:C:H2'     | 1:CA:739:C:H6      | 1.78                     | 0.49              |
| 1:CA:946:A:H3'     | 1:CA:947:G:H8      | 1.77                     | 0.49              |
| 1:CA:979:C:C3'     | 1:CA:980:C:C5'     | 2.78                     | 0.49              |
| 1:CA:995:C:O2'     | 1:CA:996:A:H5'     | 2.12                     | 0.49              |
| 5:CE:150:ARG:HB2   | 5:CE:150:ARG:NH1   | 2.28                     | 0.49              |
| 9:CI:10:ARG:CZ     | 9:CI:105:ASP:OD2   | 2.61                     | 0.49              |
| 9:CI:26:VAL:CG2    | 9:CI:61:ALA:HB3    | 2.40                     | 0.49              |
| 10:CJ:55:LYS:N     | 10:CJ:55:LYS:HE3   | 2.26                     | 0.49              |
| 1:CA:502:G:OP1     | 12:CL:118:SER:HB3  | 2.12                     | 0.49              |
| 12:CL:17:LYS:HD3   | 12:CL:18:VAL:N     | 2.28                     | 0.49              |
| 12:CL:70:ILE:HG21  | 12:CL:77:LEU:HD12  | 1.95                     | 0.49              |
| 16:CP:67:THR:N     | 16:CP:70:ALA:HB3   | 2.28                     | 0.49              |
| 24:CY:25:LYS:HG3   | 62:CY:703:GDP:O1B  | 2.12                     | 0.49              |
| 26:D1:63:ALA:O     | 26:D1:67:ILE:HG13  | 2.13                     | 0.49              |
| 31:D6:22:ALA:C     | 31:D6:23:THR:HG23  | 2.33                     | 0.49              |
| 31:D6:25:LYS:HE2   | 33:D8:34:TRP:HE1   | 1.77                     | 0.49              |
| 35:DA:1064:C:H42   | 35:DA:1074:G:H1    | 1.60                     | 0.49              |
| 35:DA:112:U:H2'    | 35:DA:113:G:H5'    | 1.95                     | 0.49              |
| 35:DA:1188:U:C2'   | 35:DA:1189:A:H5'   | 2.43                     | 0.49              |
| 35:DA:1678:G:N2    | 35:DA:1989:G:N2    | 2.53                     | 0.49              |
| 35:DA:2016:U:O2'   | 35:DA:2017:U:H5'   | 2.13                     | 0.49              |
| 35:DA:2308:G:N7    | 35:DA:2310:A:C5'   | 2.69                     | 0.49              |
| 31:D6:54:ILE:HD13  | 35:DA:2420:C:H5'   | 1.94                     | 0.49              |
| 35:DA:884:C:N4     | 35:DA:886:C:H42    | 2.11                     | 0.49              |
| 35:DA:925:C:C3'    | 35:DA:926:A:H5''   | 2.42                     | 0.49              |
| 36:DB:53:A:H2'     | 36:DB:53:A:N3      | 2.27                     | 0.49              |
| 36:DB:95:C:O2'     | 36:DB:96:U:H5'     | 2.12                     | 0.49              |
| 37:DC:128:LEU:CD1  | 37:DC:132:LEU:HG   | 2.41                     | 0.49              |
| 39:DE:14:ILE:HG13  | 39:DE:21:VAL:CG2   | 2.43                     | 0.49              |
| 41:DG:107:LEU:HD21 | 41:DG:178:PHE:CE1  | 2.48                     | 0.49              |
| 41:DG:19:LEU:HD11  | 41:DG:172:LEU:HD12 | 1.95                     | 0.49              |
| 35:DA:1081:U:O3'   | 44:DK:117:THR:HG22 | 2.12                     | 0.49              |
| 44:DK:77:LEU:CD2   | 44:DK:77:LEU:H     | 2.08                     | 0.49              |
| 49:DQ:2:LEU:HG     | 49:DQ:69:PHE:CE1   | 2.48                     | 0.49              |
| 53:DU:26:GLY:C     | 53:DU:28:ARG:N     | 2.66                     | 0.49              |
| 56:DX:68:ARG:HD3   | 56:DX:68:ARG:O     | 2.13                     | 0.49              |
| 58:DZ:103:ARG:HD2  | 58:DZ:136:PHE:CE1  | 2.48                     | 0.49              |
| 58:DZ:61:LEU:HD12  | 58:DZ:65:GLN:CB    | 2.42                     | 0.49              |
| 1:AA:1065:U:C2'    | 1:AA:1066:C:OP2    | 2.61                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1226:C:H5''   | 13:AM:103:THR:OG1  | 2.13                     | 0.49              |
| 1:AA:1258:G:C6     | 1:AA:1259:C:N4     | 2.81                     | 0.49              |
| 1:AA:1468:A:H2'    | 1:AA:1469:G:O4'    | 2.12                     | 0.49              |
| 1:AA:170:U:O2'     | 1:AA:171:A:H5'     | 2.13                     | 0.49              |
| 1:AA:344:A:H5''    | 1:AA:345:C:OP2     | 2.13                     | 0.49              |
| 1:AA:1104:G:P      | 2:AB:111:ARG:HD2   | 2.53                     | 0.49              |
| 2:AB:121:LEU:HD21  | 2:AB:126:GLU:OE2   | 2.13                     | 0.49              |
| 3:AC:151:VAL:HG12  | 3:AC:152:ILE:N     | 2.26                     | 0.49              |
| 5:AE:144:THR:O     | 5:AE:146:ALA:N     | 2.45                     | 0.49              |
| 7:AG:116:ALA:O     | 7:AG:120:ILE:HG12  | 2.12                     | 0.49              |
| 1:AA:529:G:O6      | 12:AL:49:ASN:HA    | 2.13                     | 0.49              |
| 17:AQ:94:ASN:O     | 17:AQ:95:TYR:C     | 2.49                     | 0.49              |
| 23:AX:11:U:C2'     | 23:AX:11:U:O2      | 2.60                     | 0.49              |
| 24:AY:122:TRP:O    | 24:AY:125:ALA:N    | 2.29                     | 0.49              |
| 24:AY:232:LEU:HD22 | 24:AY:232:LEU:N    | 2.26                     | 0.49              |
| 24:AY:406:GLU:CB   | 24:AY:407:PRO:HD2  | 2.42                     | 0.49              |
| 24:AY:451:ILE:HG23 | 24:AY:459:LEU:HD23 | 1.95                     | 0.49              |
| 24:AY:84:THR:O     | 24:AY:85:PRO:O     | 2.30                     | 0.49              |
| 31:B6:42:TRP:HA    | 31:B6:42:TRP:HE3   | 1.77                     | 0.49              |
| 35:BA:1141:U:OP2   | 46:BN:63:THR:OG1   | 2.24                     | 0.49              |
| 35:BA:1168:G:H2'   | 35:BA:1169:G:H8    | 1.74                     | 0.49              |
| 35:BA:1344:G:H1    | 35:BA:1403:C:H42   | 1.60                     | 0.49              |
| 35:BA:1692:U:H2'   | 35:BA:1694:C:C4    | 2.48                     | 0.49              |
| 35:BA:2156:G:H2'   | 35:BA:2157:G:O4'   | 2.13                     | 0.49              |
| 35:BA:250:G:H2'    | 35:BA:251:A:C8     | 2.47                     | 0.49              |
| 35:BA:2860:A:C2'   | 35:BA:2861:G:H5'   | 2.43                     | 0.49              |
| 35:BA:52:A:C2'     | 35:BA:53:A:H5'     | 2.43                     | 0.49              |
| 35:BA:657:U:H2'    | 35:BA:658:C:H6     | 1.74                     | 0.49              |
| 41:BG:31:VAL:HG23  | 41:BG:32:PRO:HD2   | 1.95                     | 0.49              |
| 41:BG:55:LYS:C     | 41:BG:57:ALA:N     | 2.66                     | 0.49              |
| 42:BH:46:GLU:HG3   | 42:BH:51:ARG:H     | 1.78                     | 0.49              |
| 46:BN:115:ARG:HA   | 46:BN:118:LYS:HE2  | 1.94                     | 0.49              |
| 58:BZ:120:ILE:O    | 58:BZ:120:ILE:CG2  | 2.60                     | 0.49              |
| 58:BZ:115:GLY:HA2  | 58:BZ:177:PRO:CD   | 2.43                     | 0.49              |
| 58:BZ:89:PHE:CE1   | 58:BZ:96:VAL:HG21  | 2.47                     | 0.49              |
| 58:BZ:9:TYR:HB3    | 58:BZ:35:ARG:NH2   | 2.27                     | 0.49              |
| 1:CA:1300:G:HO2'   | 1:CA:1301:U:P      | 2.36                     | 0.49              |
| 1:CA:1447:A:H2'    | 1:CA:1447:A:N3     | 2.26                     | 0.49              |
| 1:CA:184:G:O2'     | 1:CA:185:A:H5'     | 2.13                     | 0.49              |
| 1:CA:324:G:N2      | 1:CA:326:G:H3'     | 2.27                     | 0.49              |
| 1:CA:46:G:O2'      | 1:CA:365:U:H1'     | 2.13                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:CA:64:G:N2      | 1:CA:67:C:C4        | 2.81                     | 0.49              |
| 2:CB:148:TYR:O    | 2:CB:149:LEU:HD23   | 2.12                     | 0.49              |
| 2:CB:223:ILE:O    | 2:CB:225:ALA:N      | 2.45                     | 0.49              |
| 10:CJ:63:PHE:CD2  | 10:CJ:63:PHE:N      | 2.81                     | 0.49              |
| 12:CL:47:LYS:CB   | 12:CL:48:PRO:CD     | 2.89                     | 0.49              |
| 20:CT:96:GLY:O    | 20:CT:97:ALA:O      | 2.31                     | 0.49              |
| 22:CV:36:U:H1'    | 24:CY:503:GLY:H     | 1.78                     | 0.49              |
| 24:CY:513:LYS:CB  | 24:CY:566:THR:HB    | 2.43                     | 0.49              |
| 26:D1:76:ARG:HH22 | 26:D1:95:LEU:HB2    | 1.77                     | 0.49              |
| 31:D6:33:LYS:HG2  | 31:D6:34:LEU:N      | 2.28                     | 0.49              |
| 35:DA:1168:G:H2'  | 35:DA:1169:G:O4'    | 2.13                     | 0.49              |
| 35:DA:1528:A:O2'  | 35:DA:1528(A):A:O5' | 2.30                     | 0.49              |
| 35:DA:2116:G:N7   | 35:DA:2117:A:C5     | 2.81                     | 0.49              |
| 35:DA:2192:G:C3'  | 35:DA:2193:G:H5''   | 2.42                     | 0.49              |
| 35:DA:2317:C:O2'  | 35:DA:2318:G:H5'    | 2.11                     | 0.49              |
| 35:DA:2845:G:O2'  | 35:DA:2846:G:H5'    | 2.13                     | 0.49              |
| 35:DA:685:A:C5    | 35:DA:774:A:C2      | 3.00                     | 0.49              |
| 39:DE:89:ASP:O    | 39:DE:90:THR:O      | 2.30                     | 0.49              |
| 46:DN:96:GLU:O    | 46:DN:100:GLU:HG3   | 2.13                     | 0.49              |
| 30:D5:55:ARG:NH1  | 50:DR:33:ARG:CD     | 2.76                     | 0.49              |
| 52:DT:62:THR:HA   | 52:DT:74:ARG:O      | 2.13                     | 0.49              |
| 57:DY:46:LYS:HB2  | 57:DY:62:GLU:HB2    | 1.94                     | 0.49              |
| 58:DZ:54:HIS:HE1  | 58:DZ:123:ASP:OD2   | 1.96                     | 0.49              |
| 1:AA:1360:A:H2'   | 1:AA:1361:G:O4'     | 2.12                     | 0.49              |
| 1:AA:1402:C:O2    | 1:AA:1500:A:N1      | 2.46                     | 0.49              |
| 1:AA:142:G:H1     | 1:AA:221:C:H42      | 1.61                     | 0.49              |
| 1:AA:265:G:O2'    | 1:AA:266:G:H5'      | 2.13                     | 0.49              |
| 2:AB:101:MET:HG2  | 2:AB:152:PHE:CE2    | 2.48                     | 0.49              |
| 2:AB:178:ARG:CG   | 2:AB:178:ARG:HH11   | 2.26                     | 0.49              |
| 7:AG:78:ARG:HE    | 7:AG:156:TRP:HB3    | 1.78                     | 0.49              |
| 8:AH:86:ILE:HG13  | 8:AH:133:LEU:HD22   | 1.93                     | 0.49              |
| 10:AJ:22:LYS:O    | 10:AJ:22:LYS:HD2    | 2.12                     | 0.49              |
| 10:AJ:94:VAL:CG1  | 10:AJ:95:GLU:N      | 2.76                     | 0.49              |
| 12:AL:46:LYS:HZ2  | 12:AL:94:PRO:HG3    | 1.78                     | 0.49              |
| 12:AL:70:ILE:HD12 | 12:AL:75:HIS:NE2    | 2.27                     | 0.49              |
| 14:AN:12:ARG:O    | 14:AN:14:PRO:CD     | 2.61                     | 0.49              |
| 14:AN:15:LYS:O    | 14:AN:16:PHE:C      | 2.50                     | 0.49              |
| 15:AO:17:ARG:NH1  | 15:AO:77:ARG:CZ     | 2.76                     | 0.49              |
| 16:AP:23:ASP:OD1  | 16:AP:24:ALA:N      | 2.45                     | 0.49              |
| 18:AR:40:LEU:C    | 18:AR:42:ARG:H      | 2.15                     | 0.49              |
| 18:AR:32:ARG:HA   | 18:AR:69:THR:HG21   | 1.95                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:AT:33:ILE:CD1   | 20:AT:63:ILE:HA    | 2.43                     | 0.49              |
| 21:AU:9:ARG:HH11   | 21:AU:22:ARG:HG3   | 1.78                     | 0.49              |
| 23:AX:11:U:H4'     | 23:AX:12:A:O5'     | 2.11                     | 0.49              |
| 23:AX:16:A:H2'     | 23:AX:17:U:H6      | 1.78                     | 0.49              |
| 24:AY:230:LYS:HB2  | 24:AY:230:LYS:NZ   | 2.28                     | 0.49              |
| 24:AY:289:ILE:O    | 24:AY:301:ILE:HG12 | 2.13                     | 0.49              |
| 24:AY:292:THR:HG23 | 24:AY:297:GLU:H    | 1.77                     | 0.49              |
| 24:AY:507:TYR:CD1  | 24:AY:507:TYR:C    | 2.86                     | 0.49              |
| 25:B0:78:TYR:N     | 25:B0:78:TYR:CD1   | 2.78                     | 0.49              |
| 26:B1:29:GLY:O     | 26:B1:31:GLY:N     | 2.46                     | 0.49              |
| 27:B2:20:GLU:O     | 27:B2:21:LEU:C     | 2.51                     | 0.49              |
| 27:B2:57:ILE:HG22  | 27:B2:61:LEU:HD12  | 1.94                     | 0.49              |
| 34:B9:26:ILE:HG22  | 34:B9:27:CYS:N     | 2.27                     | 0.49              |
| 35:BA:1019:U:H3    | 35:BA:1142(A):A:N6 | 2.11                     | 0.49              |
| 35:BA:1169:G:C2    | 35:BA:1181:C:N3    | 2.81                     | 0.49              |
| 35:BA:1461:G:H2'   | 35:BA:1462:C:H6    | 1.77                     | 0.49              |
| 35:BA:1499:C:O2'   | 35:BA:1500:G:H5'   | 2.13                     | 0.49              |
| 35:BA:2305:A:O2'   | 41:BG:136:ARG:HG2  | 2.13                     | 0.49              |
| 35:BA:272(D):G:H1  | 35:BA:364:C:H42    | 1.61                     | 0.49              |
| 35:BA:825:C:H2'    | 35:BA:826:U:O4'    | 2.13                     | 0.49              |
| 35:BA:979:G:H2'    | 35:BA:982:C:N4     | 2.27                     | 0.49              |
| 36:BB:8:U:H5'      | 36:BB:8:U:H6       | 1.78                     | 0.49              |
| 35:BA:1568:G:P     | 38:BD:63:ARG:HH22  | 2.34                     | 0.49              |
| 41:BG:103:LEU:HA   | 41:BG:106:LEU:HB3  | 1.94                     | 0.49              |
| 42:BH:17:VAL:HB    | 42:BH:45:VAL:HG13  | 1.93                     | 0.49              |
| 44:BK:17:ALA:HB1   | 44:BK:38:VAL:HG22  | 1.91                     | 0.49              |
| 48:BP:85:LEU:HD12  | 48:BP:120:ALA:CB   | 2.32                     | 0.49              |
| 1:AA:1442:G:H2'    | 52:BT:118:ARG:HH12 | 1.77                     | 0.49              |
| 35:BA:2019:A:O3'   | 53:BU:27:LEU:HD12  | 2.12                     | 0.49              |
| 55:BW:82:LEU:N     | 55:BW:82:LEU:CD1   | 2.76                     | 0.49              |
| 57:BY:29:GLU:N     | 57:BY:29:GLU:OE1   | 2.46                     | 0.49              |
| 1:CA:1216:G:H2'    | 1:CA:1217:C:C6     | 2.48                     | 0.49              |
| 1:CA:190:U:O2'     | 1:CA:191:G:H5'     | 2.13                     | 0.49              |
| 1:CA:218:C:H5'     | 1:CA:470:C:H41     | 1.78                     | 0.49              |
| 1:CA:409:G:H1      | 1:CA:433:C:H42     | 1.61                     | 0.49              |
| 1:CA:624:C:H2'     | 1:CA:625:G:C8      | 2.48                     | 0.49              |
| 1:CA:858:G:O2'     | 1:CA:859:A:H5''    | 2.13                     | 0.49              |
| 2:CB:109:SER:O     | 2:CB:112:VAL:HB    | 2.13                     | 0.49              |
| 3:CC:173:VAL:O     | 3:CC:175:LEU:HD12  | 2.12                     | 0.49              |
| 4:CD:31:CYS:O      | 4:CD:32:ALA:CB     | 2.60                     | 0.49              |
| 6:CF:33:TYR:O      | 6:CF:34:GLY:C      | 2.51                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:CH:104:ARG:O     | 8:CH:105:ARG:C     | 2.51                     | 0.49              |
| 1:CA:1226:C:H5''   | 13:CM:103:THR:HB   | 1.94                     | 0.49              |
| 18:CR:53:ARG:C     | 18:CR:55:ARG:N     | 2.66                     | 0.49              |
| 19:CS:31:ILE:O     | 19:CS:31:ILE:HG23  | 2.12                     | 0.49              |
| 22:CW:18:U:H2'     | 22:CW:18:U:O2      | 2.13                     | 0.49              |
| 24:CY:102:ASP:O    | 24:CY:130:VAL:HG22 | 2.12                     | 0.49              |
| 24:CY:272:LEU:HD12 | 24:CY:275:ALA:HB3  | 1.95                     | 0.49              |
| 24:CY:34:TYR:CD2   | 24:CY:35:TYR:HE2   | 2.30                     | 0.49              |
| 24:CY:326:THR:OG1  | 24:CY:377:VAL:HG22 | 2.13                     | 0.49              |
| 24:CY:456:GLU:O    | 24:CY:460:GLU:HB2  | 2.12                     | 0.49              |
| 24:CY:670:VAL:O    | 24:CY:671:MET:HB3  | 2.12                     | 0.49              |
| 24:CY:92:ILE:HG21  | 24:CY:454:MET:HE1  | 1.95                     | 0.49              |
| 26:D1:30:VAL:CG2   | 26:D1:31:GLY:H     | 2.24                     | 0.49              |
| 33:D8:21:LYS:HD3   | 33:D8:48:PHE:CE2   | 2.48                     | 0.49              |
| 35:DA:324:A:OP2    | 35:DA:1205:U:N3    | 2.46                     | 0.49              |
| 30:D5:24:ALA:HB2   | 35:DA:15:G:OP1     | 2.12                     | 0.49              |
| 35:DA:2020:A:C6    | 35:DA:2022:U:N3    | 2.81                     | 0.49              |
| 35:DA:2223:G:C2'   | 35:DA:2224:G:H5'   | 2.43                     | 0.49              |
| 35:DA:2320:A:C2    | 35:DA:2333:A:C8    | 3.01                     | 0.49              |
| 35:DA:2892:A:H62   | 35:DA:2893:G:H21   | 1.59                     | 0.49              |
| 35:DA:29:U:O2'     | 35:DA:30:G:H5'     | 2.12                     | 0.49              |
| 35:DA:325:G:H2'    | 35:DA:326:G:H8     | 1.78                     | 0.49              |
| 36:DB:86:G:C6      | 36:DB:92:C:N3      | 2.81                     | 0.49              |
| 37:DC:138:LEU:HD13 | 37:DC:138:LEU:C    | 2.33                     | 0.49              |
| 38:DD:14:ARG:HG3   | 38:DD:15:PHE:N     | 2.28                     | 0.49              |
| 38:DD:200:ASP:O    | 38:DD:201:HIS:C    | 2.51                     | 0.49              |
| 39:DE:69:LYS:O     | 39:DE:71:GLY:N     | 2.45                     | 0.49              |
| 40:DF:107:LYS:O    | 40:DF:108:LYS:C    | 2.51                     | 0.49              |
| 46:DN:133:GLN:O    | 46:DN:134:ARG:HB3  | 2.13                     | 0.49              |
| 52:DT:50:ILE:CG1   | 52:DT:102:ILE:HD11 | 2.42                     | 0.49              |
| 53:DU:55:ARG:HA    | 53:DU:58:ARG:HB2   | 1.95                     | 0.49              |
| 53:DU:59:ARG:O     | 53:DU:62:ILE:N     | 2.42                     | 0.49              |
| 54:DV:38:LEU:C     | 54:DV:39:LEU:HD13  | 2.33                     | 0.49              |
| 35:DA:2012:G:C4'   | 55:DW:96:ILE:HD11  | 2.18                     | 0.49              |
| 57:DY:46:LYS:H     | 57:DY:62:GLU:CB    | 2.19                     | 0.49              |
| 57:DY:49:VAL:O     | 57:DY:51:VAL:HG23  | 2.12                     | 0.49              |
| 44:DK:93:ARG:CG    | 58:DZ:112:ARG:HE   | 2.26                     | 0.49              |
| 58:DZ:128:VAL:CG2  | 58:DZ:129:SER:H    | 2.23                     | 0.49              |
| 1:AA:1225:A:H3'    | 1:AA:1226:C:C6     | 2.48                     | 0.49              |
| 1:AA:1277:C:H3'    | 1:AA:1277:C:H6     | 1.77                     | 0.49              |
| 1:AA:1301:U:H3'    | 1:AA:1302:U:H5''   | 1.94                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:253:U:H2'     | 1:AA:254:G:H8      | 1.77                     | 0.49              |
| 1:AA:318:G:H2'     | 1:AA:319:G:H8      | 1.77                     | 0.49              |
| 1:AA:63:C:O2'      | 1:AA:380:G:H4'     | 2.13                     | 0.49              |
| 2:AB:15:VAL:H      | 2:AB:16:HIS:CE1    | 2.31                     | 0.49              |
| 3:AC:10:PHE:CE1    | 3:AC:178:LEU:HD11  | 2.48                     | 0.49              |
| 4:AD:31:CYS:O      | 4:AD:32:ALA:CB     | 2.60                     | 0.49              |
| 5:AE:51:VAL:HB     | 5:AE:52:PRO:CD     | 2.41                     | 0.49              |
| 5:AE:68:GLU:O      | 5:AE:68:GLU:HG3    | 2.13                     | 0.49              |
| 7:AG:134:ALA:O     | 7:AG:137:LYS:N     | 2.42                     | 0.49              |
| 9:AI:59:PHE:CD1    | 9:AI:59:PHE:N      | 2.81                     | 0.49              |
| 19:AS:35:SER:C     | 19:AS:37:ARG:N     | 2.66                     | 0.49              |
| 24:AY:413:ILE:O    | 24:AY:413:ILE:HG23 | 2.13                     | 0.49              |
| 24:AY:519:ARG:HH21 | 24:AY:677:GLN:HB2  | 1.78                     | 0.49              |
| 24:AY:679:VAL:HG23 | 24:AY:684:GLN:NE2  | 2.28                     | 0.49              |
| 25:B0:47:PRO:HB3   | 25:B0:51:VAL:O     | 2.12                     | 0.49              |
| 28:B3:2:PRO:O      | 28:B3:3:ARG:O      | 2.31                     | 0.49              |
| 35:BA:1040:C:H2'   | 35:BA:1041:C:C6    | 2.47                     | 0.49              |
| 35:BA:1441:G:O2'   | 35:BA:1442:G:H5'   | 2.13                     | 0.49              |
| 35:BA:1462:C:H4'   | 35:BA:2703:C:H5'   | 1.94                     | 0.49              |
| 35:BA:1582:C:H2'   | 35:BA:1583:A:C8    | 2.43                     | 0.49              |
| 35:BA:194:G:H2'    | 35:BA:195:A:O4'    | 2.11                     | 0.49              |
| 35:BA:1326:U:H5''  | 35:BA:2011:U:H1'   | 1.93                     | 0.49              |
| 35:BA:272(I):U:O2  | 35:BA:272(I):U:C3' | 2.59                     | 0.49              |
| 35:BA:29:U:O2'     | 35:BA:30:G:H5'     | 2.13                     | 0.49              |
| 35:BA:345:A:O2'    | 35:BA:346:A:N7     | 2.46                     | 0.49              |
| 35:BA:408:G:O2'    | 35:BA:409:C:H5'    | 2.13                     | 0.49              |
| 35:BA:478:A:C6     | 35:BA:480:A:C6     | 3.00                     | 0.49              |
| 35:BA:729:G:OP2    | 38:BD:13:ARG:NH1   | 2.46                     | 0.49              |
| 35:BA:821:A:O2'    | 35:BA:945:A:H3'    | 2.13                     | 0.49              |
| 29:B4:2:LYS:HG2    | 36:BB:44:G:P       | 2.52                     | 0.49              |
| 37:BC:115:VAL:HG12 | 37:BC:145:THR:CG2  | 2.40                     | 0.49              |
| 37:BC:23:ILE:CB    | 37:BC:229:SER:OXT  | 2.60                     | 0.49              |
| 39:BE:51:PHE:N     | 39:BE:74:PRO:HG3   | 2.28                     | 0.49              |
| 41:BG:56:ALA:CB    | 41:BG:153:ARG:NH2  | 2.76                     | 0.49              |
| 46:BN:58:ASP:C     | 46:BN:60:ILE:N     | 2.60                     | 0.49              |
| 48:BP:107:LYS:O    | 48:BP:109:GLY:N    | 2.45                     | 0.49              |
| 35:BA:2415:G:H4'   | 48:BP:66:GLY:C     | 2.33                     | 0.49              |
| 35:BA:958:U:H5'    | 49:BQ:14:ARG:NH1   | 2.27                     | 0.49              |
| 50:BR:12:ARG:HB3   | 50:BR:16:HIS:HD2   | 1.78                     | 0.49              |
| 51:BS:40:ILE:CG2   | 51:BS:41:ASP:N     | 2.76                     | 0.49              |
| 53:BU:112:ARG:CZ   | 54:BV:46:VAL:HG21  | 2.43                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:BZ:109:ALA:HB1  | 58:BZ:145:GLU:OE2  | 2.13                     | 0.49              |
| 1:CA:1346:A:N6     | 1:CA:1375:A:OP2    | 2.40                     | 0.49              |
| 1:CA:1497:G:O2'    | 1:CA:1498:U:H5'    | 2.13                     | 0.49              |
| 1:CA:1511:G:O2'    | 1:CA:1512:U:H5'    | 2.13                     | 0.49              |
| 1:CA:60:A:C5'      | 1:CA:331:G:H22     | 2.23                     | 0.49              |
| 3:CC:61:ALA:O      | 3:CC:62:ASP:HB2    | 2.12                     | 0.49              |
| 6:CF:22:GLU:HA     | 6:CF:22:GLU:OE2    | 2.12                     | 0.49              |
| 8:CH:31:PHE:O      | 8:CH:34:GLU:HB2    | 2.13                     | 0.49              |
| 14:CN:25:VAL:HG23  | 14:CN:38:GLY:O     | 2.12                     | 0.49              |
| 24:CY:105:ILE:N    | 24:CY:105:ILE:HD12 | 2.28                     | 0.49              |
| 24:CY:146:LEU:HD12 | 24:CY:167:PRO:HD3  | 1.95                     | 0.49              |
| 24:CY:451:ILE:O    | 24:CY:451:ILE:HG23 | 2.13                     | 0.49              |
| 24:CY:513:LYS:HB2  | 24:CY:566:THR:HB   | 1.95                     | 0.49              |
| 24:CY:529:ILE:HD11 | 24:CY:534:ILE:HD12 | 1.95                     | 0.49              |
| 25:D0:10:THR:HG22  | 25:D0:11:ARG:N     | 2.28                     | 0.49              |
| 27:D2:16:LEU:O     | 27:D2:20:GLU:HB3   | 2.13                     | 0.49              |
| 27:D2:53:LEU:O     | 27:D2:57:ILE:HG12  | 2.11                     | 0.49              |
| 28:D3:31:LEU:HD22  | 28:D3:32:GLN:H     | 1.77                     | 0.49              |
| 30:D5:55:ARG:O     | 30:D5:56:LYS:CB    | 2.52                     | 0.49              |
| 32:D7:28:ARG:NH1   | 32:D7:28:ARG:HG3   | 2.28                     | 0.49              |
| 35:DA:1035:U:H2'   | 35:DA:1036:G:C8    | 2.47                     | 0.49              |
| 35:DA:2453:A:OP1   | 35:DA:2573:C:H5    | 1.96                     | 0.49              |
| 35:DA:2747:G:O2'   | 42:DH:67:LEU:HD12  | 2.13                     | 0.49              |
| 35:DA:2804:C:H2'   | 35:DA:2805:G:H8    | 1.69                     | 0.49              |
| 35:DA:48:G:N2      | 35:DA:177:G:N2     | 2.61                     | 0.49              |
| 35:DA:537:C:H2'    | 35:DA:538:G:C8     | 2.48                     | 0.49              |
| 35:DA:618:C:H2'    | 35:DA:619:G:O4'    | 2.13                     | 0.49              |
| 35:DA:718:A:H2'    | 35:DA:719:C:O4'    | 2.13                     | 0.49              |
| 35:DA:756:C:C2'    | 35:DA:757:U:H5'    | 2.43                     | 0.49              |
| 35:DA:777:A:H2'    | 35:DA:778:G:C8     | 2.48                     | 0.49              |
| 35:DA:76:C:O2'     | 35:DA:77:C:H5'     | 2.13                     | 0.49              |
| 35:DA:90:U:H3'     | 35:DA:90:U:O2      | 2.13                     | 0.49              |
| 35:DA:938:G:H2'    | 35:DA:939:G:H8     | 1.77                     | 0.49              |
| 35:DA:961:C:N4     | 35:DA:2031:A:H1'   | 2.27                     | 0.49              |
| 36:DB:74:U:H2'     | 36:DB:75:G:H5'     | 1.95                     | 0.49              |
| 38:DD:81:ALA:HA    | 38:DD:113:VAL:CG2  | 2.43                     | 0.49              |
| 39:DE:152:LYS:HG3  | 39:DE:153:GLY:N    | 2.27                     | 0.49              |
| 40:DF:42:ALA:O     | 40:DF:45:ARG:HG3   | 2.12                     | 0.49              |
| 41:DG:40:ASN:O     | 41:DG:156:ASP:N    | 2.40                     | 0.49              |
| 41:DG:46:ALA:O     | 41:DG:47:LYS:O     | 2.31                     | 0.49              |
| 46:DN:133:GLN:CG   | 46:DN:134:ARG:N    | 2.75                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 46:DN:18:ALA:O     | 46:DN:21:LYS:HB2  | 2.12                     | 0.49              |
| 50:DR:63:ARG:HA    | 50:DR:80:PHE:CZ   | 2.48                     | 0.49              |
| 51:DS:89:ARG:HG3   | 51:DS:92:TYR:HB3  | 1.95                     | 0.49              |
| 52:DT:82:LEU:CD2   | 52:DT:85:LYS:HD2  | 2.43                     | 0.49              |
| 58:DZ:109:ALA:C    | 58:DZ:111:VAL:N   | 2.66                     | 0.49              |
| 58:DZ:96:VAL:O     | 58:DZ:96:VAL:HG13 | 2.11                     | 0.49              |
| 1:AA:238:G:C6      | 1:AA:239:U:C4     | 3.00                     | 0.48              |
| 1:AA:532:A:H61     | 3:AC:193:TYR:HB3  | 1.78                     | 0.48              |
| 1:AA:509:A:H2      | 1:AA:543:C:H1'    | 1.78                     | 0.48              |
| 1:AA:908:A:H2'     | 1:AA:909:A:C8     | 2.48                     | 0.48              |
| 4:AD:170:VAL:O     | 4:AD:171:GLY:O    | 2.31                     | 0.48              |
| 8:AH:30:ARG:CB     | 8:AH:30:ARG:HH11  | 2.26                     | 0.48              |
| 8:AH:32:LYS:O      | 8:AH:34:GLU:N     | 2.46                     | 0.48              |
| 8:AH:85:ARG:HG3    | 8:AH:85:ARG:HH11  | 1.77                     | 0.48              |
| 9:AI:83:ARG:O      | 9:AI:86:VAL:HG12  | 2.13                     | 0.48              |
| 10:AJ:22:LYS:NZ    | 10:AJ:88:LEU:HD23 | 2.29                     | 0.48              |
| 13:AM:79:LYS:HA    | 13:AM:82:MET:HG3  | 1.95                     | 0.48              |
| 24:AY:139:MET:CE   | 24:AY:167:PRO:HG3 | 2.42                     | 0.48              |
| 24:AY:341:VAL:HG23 | 24:AY:350:GLU:HB2 | 1.95                     | 0.48              |
| 29:B4:22:ILE:CG2   | 29:B4:23:GLU:N    | 2.76                     | 0.48              |
| 30:B5:27:PRO:CD    | 55:BW:23:LEU:HD11 | 2.43                     | 0.48              |
| 30:B5:55:ARG:NH1   | 50:BR:33:ARG:CD   | 2.75                     | 0.48              |
| 31:B6:27:LYS:CD    | 31:B6:30:THR:HB   | 2.43                     | 0.48              |
| 31:B6:47:THR:OG1   | 31:B6:48:VAL:N    | 2.46                     | 0.48              |
| 35:BA:1353:A:H4'   | 38:BD:38:LYS:HE3  | 1.95                     | 0.48              |
| 35:BA:2230:G:H2'   | 35:BA:2231:C:C6   | 2.48                     | 0.48              |
| 35:BA:2348:U:H2'   | 35:BA:2349:G:H5'  | 1.95                     | 0.48              |
| 35:BA:2367:G:H2'   | 35:BA:2368:C:H6   | 1.77                     | 0.48              |
| 35:BA:409:C:O2'    | 35:BA:410:G:H5'   | 2.13                     | 0.48              |
| 27:B2:48:HIS:HD1   | 35:BA:95:G:HO2'   | 1.58                     | 0.48              |
| 39:BE:203:LYS:HG3  | 39:BE:204:ALA:N   | 2.27                     | 0.48              |
| 39:BE:36:ARG:HH21  | 39:BE:88:GLY:HA2  | 1.77                     | 0.48              |
| 41:BG:110:ALA:HA   | 41:BG:140:ILE:O   | 2.13                     | 0.48              |
| 41:BG:165:THR:O    | 41:BG:166:ASP:C   | 2.50                     | 0.48              |
| 41:BG:97:ASP:O     | 41:BG:101:ILE:N   | 2.42                     | 0.48              |
| 47:BO:98:VAL:CG2   | 47:BO:118:ALA:HA  | 2.43                     | 0.48              |
| 48:BP:16:ARG:CZ    | 48:BP:18:ARG:HB2  | 2.43                     | 0.48              |
| 48:BP:64:LYS:O     | 48:BP:64:LYS:HD3  | 2.13                     | 0.48              |
| 49:BQ:134:ARG:HH11 | 49:BQ:134:ARG:HG3 | 1.78                     | 0.48              |
| 35:BA:910:A:C6     | 49:BQ:13:GLN:HG3  | 2.48                     | 0.48              |
| 49:BQ:11:LYS:NZ    | 49:BQ:88:GLY:O    | 2.40                     | 0.48              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:BS:33:LYS:HG2   | 51:BS:34:HIS:CD2   | 2.48                     | 0.48              |
| 52:BT:62:THR:HA    | 52:BT:74:ARG:O     | 2.13                     | 0.48              |
| 57:BY:31:LEU:HD22  | 57:BY:31:LEU:H     | 1.77                     | 0.48              |
| 1:CA:1296:C:O2'    | 1:CA:1302:U:C5     | 2.60                     | 0.48              |
| 1:CA:965:A:C2      | 1:CA:969:A:C2      | 3.01                     | 0.48              |
| 1:CA:973:G:O4'     | 10:CJ:55:LYS:HE2   | 2.13                     | 0.48              |
| 1:CA:986:A:H2'     | 1:CA:987:G:H8      | 1.78                     | 0.48              |
| 10:CJ:42:THR:HG23  | 10:CJ:67:THR:O     | 2.12                     | 0.48              |
| 19:CS:19:VAL:HG12  | 19:CS:20:LEU:HG    | 1.95                     | 0.48              |
| 22:CV:57:A:H2'     | 22:CV:58:A:H5'     | 1.95                     | 0.48              |
| 24:CY:192:LEU:HD12 | 24:CY:194:THR:HG23 | 1.94                     | 0.48              |
| 24:CY:122:TRP:HH2  | 24:CY:256:THR:OG1  | 1.96                     | 0.48              |
| 24:CY:35:TYR:O     | 24:CY:36:THR:C     | 2.50                     | 0.48              |
| 24:CY:423:LYS:NZ   | 24:CY:470:PHE:O    | 2.38                     | 0.48              |
| 29:D4:22:ILE:CG2   | 29:D4:23:GLU:N     | 2.76                     | 0.48              |
| 30:D5:19:ARG:HD2   | 35:DA:1266:G:OP1   | 2.13                     | 0.48              |
| 30:D5:35:GLU:O     | 30:D5:36:CYS:CB    | 2.60                     | 0.48              |
| 35:DA:1047:G:O2'   | 35:DA:1110:G:N2    | 2.45                     | 0.48              |
| 35:DA:1175:U:H4'   | 35:DA:1176:G:H5'   | 1.95                     | 0.48              |
| 35:DA:1558:A:O2'   | 35:DA:1559:G:OP2   | 2.30                     | 0.48              |
| 35:DA:2656:U:N3    | 35:DA:2665:A:H2    | 2.11                     | 0.48              |
| 35:DA:2794:C:H42   | 35:DA:2801(A):A:N6 | 2.11                     | 0.48              |
| 41:DG:126:ASP:CB   | 41:DG:130:ASN:HB2  | 2.42                     | 0.48              |
| 43:DJ:18:UNK:O     | 43:DJ:88:UNK:CB    | 2.61                     | 0.48              |
| 48:DP:95:VAL:CG2   | 48:DP:125:VAL:HG23 | 2.42                     | 0.48              |
| 48:DP:112:LEU:H    | 48:DP:128:HIS:HD2  | 1.58                     | 0.48              |
| 1:AA:1222:G:O2'    | 1:AA:1223:C:H5'    | 2.13                     | 0.48              |
| 1:AA:1300:G:HO2'   | 1:AA:1301:U:P      | 2.34                     | 0.48              |
| 1:AA:1366:C:H2'    | 1:AA:1367:C:C6     | 2.49                     | 0.48              |
| 1:AA:1377:A:H2'    | 7:AG:7:ALA:HB2     | 1.95                     | 0.48              |
| 1:AA:1479:C:O2'    | 1:AA:1480:G:H5'    | 2.13                     | 0.48              |
| 1:AA:409:G:H1      | 1:AA:433:C:H42     | 1.60                     | 0.48              |
| 4:AD:96:LEU:N      | 4:AD:96:LEU:HD22   | 2.23                     | 0.48              |
| 10:AJ:27:ALA:CB    | 10:AJ:85:LEU:HD11  | 2.43                     | 0.48              |
| 19:AS:42:PRO:C     | 19:AS:43:GLU:HG3   | 2.33                     | 0.48              |
| 20:AT:26:ASN:ND2   | 20:AT:26:ASN:N     | 2.61                     | 0.48              |
| 25:B0:5:LYS:HB3    | 25:B0:5:LYS:NZ     | 2.29                     | 0.48              |
| 30:B5:2:ALA:CA     | 35:BA:2015:A:C1'   | 2.86                     | 0.48              |
| 32:B7:34:ARG:HH12  | 32:B7:39:ARG:CD    | 2.26                     | 0.48              |
| 32:B7:8:ASN:HD22   | 32:B7:9:ARG:H      | 1.60                     | 0.48              |
| 35:BA:1270:C:H5''  | 35:BA:1271:G:O5'   | 2.13                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:1767:C:H2'   | 35:BA:1768:U:O4'   | 2.13                     | 0.48              |
| 35:BA:2053:G:H1    | 35:BA:2616:C:H42   | 1.60                     | 0.48              |
| 35:BA:2115:G:H3'   | 35:BA:2116:G:C5'   | 2.43                     | 0.48              |
| 35:BA:2135:A:H2'   | 35:BA:2136:C:O4'   | 2.13                     | 0.48              |
| 35:BA:229:A:H8     | 35:BA:229:A:OP1    | 1.96                     | 0.48              |
| 35:BA:2470:G:C6    | 35:BA:2471:C:C5    | 3.01                     | 0.48              |
| 35:BA:247:G:H4'    | 35:BA:386:G:C5     | 2.48                     | 0.48              |
| 35:BA:618:C:H2'    | 35:BA:619:G:O4'    | 2.13                     | 0.48              |
| 35:BA:68:G:H2'     | 35:BA:69:C:C6      | 2.47                     | 0.48              |
| 37:BC:11:LEU:C     | 37:BC:13:GLU:N     | 2.66                     | 0.48              |
| 38:BD:4:LYS:NZ     | 38:BD:21:PHE:H     | 2.11                     | 0.48              |
| 42:BH:156:ALA:C    | 42:BH:158:HIS:H    | 2.16                     | 0.48              |
| 42:BH:171:LEU:HD23 | 42:BH:172:LYS:N    | 2.28                     | 0.48              |
| 44:BK:2:LYS:HB2    | 44:BK:2:LYS:NZ     | 2.28                     | 0.48              |
| 46:BN:67:LEU:HB3   | 46:BN:88:GLU:HG2   | 1.93                     | 0.48              |
| 48:BP:124:LYS:HD3  | 48:BP:143:GLY:CA   | 2.43                     | 0.48              |
| 49:BQ:58:PHE:CD1   | 49:BQ:58:PHE:O     | 2.66                     | 0.48              |
| 52:BT:113:LYS:O    | 52:BT:114:LEU:HD23 | 2.13                     | 0.48              |
| 52:BT:6:LEU:O      | 52:BT:7:ILE:C      | 2.51                     | 0.48              |
| 53:BU:84:LYS:C     | 53:BU:86:ALA:H     | 2.15                     | 0.48              |
| 58:BZ:26:GLY:O     | 58:BZ:27:VAL:HB    | 2.13                     | 0.48              |
| 1:CA:1485:U:O2'    | 1:CA:1486:G:H5'    | 2.12                     | 0.48              |
| 1:CA:814:A:H5'     | 1:CA:1511:G:H4'    | 1.95                     | 0.48              |
| 1:CA:201:C:C2'     | 1:CA:202:U:H5''    | 2.43                     | 0.48              |
| 1:CA:542:G:H5'     | 4:CD:41:GLY:HA2    | 1.95                     | 0.48              |
| 1:CA:63:C:O2'      | 1:CA:380:G:H4'     | 2.13                     | 0.48              |
| 1:CA:6:G:H2'       | 5:CE:119:LEU:CD1   | 2.44                     | 0.48              |
| 1:CA:908:A:H2'     | 1:CA:909:A:C8      | 2.48                     | 0.48              |
| 2:CB:137:ARG:HH11  | 2:CB:137:ARG:HG2   | 1.77                     | 0.48              |
| 3:CC:59:ARG:HG2    | 3:CC:64:VAL:HA     | 1.95                     | 0.48              |
| 1:CA:1298:C:H5''   | 7:CG:114:ARG:NH2   | 2.28                     | 0.48              |
| 8:CH:123:GLU:O     | 8:CH:126:LYS:HB3   | 2.12                     | 0.48              |
| 10:CJ:4:ILE:CD1    | 10:CJ:74:ILE:HG13  | 2.39                     | 0.48              |
| 13:CM:45:VAL:HA    | 13:CM:48:LEU:CD1   | 2.44                     | 0.48              |
| 1:CA:1216:G:OP1    | 14:CN:2:ALA:HA     | 2.12                     | 0.48              |
| 15:CO:53:HIS:O     | 15:CO:56:LEU:HB3   | 2.13                     | 0.48              |
| 16:CP:13:HIS:C     | 16:CP:15:PRO:HD3   | 2.33                     | 0.48              |
| 16:CP:54:GLU:OE2   | 16:CP:54:GLU:HA    | 2.13                     | 0.48              |
| 17:CQ:94:ASN:O     | 17:CQ:96:GLU:N     | 2.46                     | 0.48              |
| 19:CS:41:VAL:C     | 19:CS:43:GLU:N     | 2.66                     | 0.48              |
| 19:CS:51:VAL:HG22  | 19:CS:71:LEU:HD13  | 1.94                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:CT:74:LYS:H     | 20:CT:74:LYS:HD3   | 1.77                     | 0.48              |
| 22:CW:36:A:O2'     | 22:CW:37:U:H5'     | 2.14                     | 0.48              |
| 22:CW:2:G:H2'      | 22:CW:3:C:C6       | 2.48                     | 0.48              |
| 24:CY:9:LEU:CD2    | 24:CY:284:LEU:HB2  | 2.43                     | 0.48              |
| 26:D1:29:GLY:O     | 26:D1:31:GLY:N     | 2.46                     | 0.48              |
| 27:D2:16:LEU:O     | 27:D2:20:GLU:CB    | 2.61                     | 0.48              |
| 31:D6:6:ARG:O      | 31:D6:7:ILE:CB     | 2.61                     | 0.48              |
| 35:DA:1233:C:H2'   | 35:DA:1234:U:H6    | 1.76                     | 0.48              |
| 35:DA:1767:C:H2'   | 35:DA:1768:U:O4'   | 2.13                     | 0.48              |
| 35:DA:2293:C:OP1   | 51:DS:92:TYR:OH    | 2.31                     | 0.48              |
| 36:DB:68:C:H2'     | 36:DB:69:G:C8      | 2.48                     | 0.48              |
| 36:DB:8:U:H5'      | 36:DB:8:U:H6       | 1.78                     | 0.48              |
| 38:DD:267:SER:C    | 38:DD:269:PHE:H    | 2.17                     | 0.48              |
| 39:DE:87:GLU:O     | 39:DE:89:ASP:N     | 2.46                     | 0.48              |
| 39:DE:36:ARG:NH2   | 39:DE:88:GLY:CA    | 2.75                     | 0.48              |
| 40:DF:199:TRP:O    | 40:DF:202:PHE:HB3  | 2.13                     | 0.48              |
| 40:DF:62:ARG:NH2   | 40:DF:64:ILE:HA    | 2.28                     | 0.48              |
| 42:DH:146:ALA:O    | 42:DH:149:ARG:N    | 2.46                     | 0.48              |
| 42:DH:17:VAL:O     | 42:DH:45:VAL:CG2   | 2.60                     | 0.48              |
| 24:CY:231:TYR:HE2  | 45:DL:87:UNK:CB    | 2.26                     | 0.48              |
| 46:DN:126:PRO:O    | 46:DN:127:ASP:CB   | 2.60                     | 0.48              |
| 46:DN:132:ALA:O    | 46:DN:133:GLN:CB   | 2.61                     | 0.48              |
| 48:DP:107:LYS:C    | 48:DP:109:GLY:N    | 2.66                     | 0.48              |
| 48:DP:146:VAL:HG13 | 48:DP:147:LEU:N    | 2.27                     | 0.48              |
| 49:DQ:68:ILE:HG23  | 49:DQ:103:MET:HA   | 1.94                     | 0.48              |
| 30:D5:55:ARG:NH1   | 50:DR:33:ARG:HD2   | 2.28                     | 0.48              |
| 51:DS:35:ILE:CD1   | 51:DS:99:LYS:HE3   | 2.42                     | 0.48              |
| 52:DT:91:ARG:O     | 52:DT:117:ASP:CB   | 2.61                     | 0.48              |
| 54:DV:2:PHE:O      | 54:DV:14:VAL:O     | 2.31                     | 0.48              |
| 57:DY:52:SER:N     | 57:DY:53:PRO:CD    | 2.76                     | 0.48              |
| 58:DZ:165:VAL:HG12 | 58:DZ:166:SER:N    | 2.29                     | 0.48              |
| 1:AA:1344:C:O2'    | 1:AA:1345:U:H5'    | 2.12                     | 0.48              |
| 2:AB:60:ASP:O      | 2:AB:64:ARG:NE     | 2.46                     | 0.48              |
| 2:AB:7:VAL:C       | 2:AB:11:LEU:HG     | 2.33                     | 0.48              |
| 3:AC:126:ARG:HD2   | 3:AC:128:PHE:CZ    | 2.48                     | 0.48              |
| 3:AC:127:ARG:HH11  | 3:AC:127:ARG:HG2   | 1.78                     | 0.48              |
| 10:AJ:40:LEU:CB    | 10:AJ:41:PRO:HD2   | 2.44                     | 0.48              |
| 20:AT:84:LEU:O     | 20:AT:86:ARG:N     | 2.46                     | 0.48              |
| 24:AY:122:TRP:CZ2  | 24:AY:159:ALA:HB2  | 2.49                     | 0.48              |
| 24:AY:25:LYS:NZ    | 24:AY:86:GLY:HA2   | 2.27                     | 0.48              |
| 24:AY:77:HIS:CD2   | 24:AY:277:VAL:HG21 | 2.48                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:AY:303:PRO:HA   | 24:AY:331:TYR:O    | 2.12                     | 0.48              |
| 24:AY:314:PHE:CD1  | 24:AY:315:LYS:HB2  | 2.48                     | 0.48              |
| 24:AY:518:PRO:HD2  | 24:AY:521:SER:OG   | 2.13                     | 0.48              |
| 24:AY:561:VAL:O    | 24:AY:562:ASP:HB2  | 2.13                     | 0.48              |
| 24:AY:510:VAL:HG11 | 24:AY:567:LEU:HD13 | 1.96                     | 0.48              |
| 31:B6:11:LEU:C     | 31:B6:11:LEU:HD22  | 2.33                     | 0.48              |
| 35:BA:1028:A:H61   | 35:BA:1125:G:H2'   | 1.77                     | 0.48              |
| 35:BA:1047:G:O2'   | 35:BA:1110:G:N2    | 2.46                     | 0.48              |
| 35:BA:688:U:C4'    | 35:BA:1780:A:C2    | 2.97                     | 0.48              |
| 35:BA:2182:G:H2'   | 35:BA:2183:C:C6    | 2.48                     | 0.48              |
| 35:BA:2205:C:H2'   | 35:BA:2205:C:O2    | 2.12                     | 0.48              |
| 35:BA:2678:C:O2'   | 35:BA:2679:A:H5'   | 2.14                     | 0.48              |
| 35:BA:2754:U:H2'   | 35:BA:2756:U:OP1   | 2.12                     | 0.48              |
| 35:BA:295:G:O2'    | 35:BA:296:C:H5'    | 2.13                     | 0.48              |
| 35:BA:428:A:H3'    | 35:BA:429:A:C8     | 2.47                     | 0.48              |
| 35:BA:90:U:H3'     | 35:BA:90:U:O2      | 2.13                     | 0.48              |
| 35:BA:938:G:H2'    | 35:BA:939:G:H8     | 1.78                     | 0.48              |
| 35:BA:999:U:OP2    | 35:BA:1153:C:OP2   | 2.31                     | 0.48              |
| 38:BD:183:ARG:CG   | 38:BD:183:ARG:HH11 | 2.14                     | 0.48              |
| 38:BD:259:THR:O    | 38:BD:260:ARG:O    | 2.32                     | 0.48              |
| 38:BD:43:ARG:HB3   | 38:BD:54:ARG:CB    | 2.42                     | 0.48              |
| 38:BD:77:ALA:O     | 38:BD:116:GLN:HG3  | 2.12                     | 0.48              |
| 40:BF:150:GLY:HA2  | 40:BF:172:TRP:CE3  | 2.49                     | 0.48              |
| 35:BA:443:A:H3'    | 40:BF:45:ARG:NH2   | 2.27                     | 0.48              |
| 41:BG:46:ALA:C     | 41:BG:51:ARG:HG3   | 2.34                     | 0.48              |
| 44:BK:121:GLU:O    | 44:BK:125:ARG:HG3  | 2.13                     | 0.48              |
| 49:BQ:45:GLN:H     | 49:BQ:45:GLN:HE21  | 1.54                     | 0.48              |
| 55:BW:41:LYS:C     | 55:BW:43:GLY:N     | 2.66                     | 0.48              |
| 56:BX:7:VAL:HB     | 56:BX:8:ILE:HD12   | 1.95                     | 0.48              |
| 58:BZ:151:HIS:O    | 58:BZ:152:ALA:C    | 2.51                     | 0.48              |
| 58:BZ:9:TYR:HE2    | 58:BZ:61:LEU:HD13  | 1.77                     | 0.48              |
| 58:BZ:92:SER:HB2   | 58:BZ:93:ASP:H     | 1.36                     | 0.48              |
| 1:CA:1405:G:H21    | 1:CA:1518:A:H1'    | 1.77                     | 0.48              |
| 1:CA:1444:C:O5'    | 1:CA:1444:C:H6     | 1.96                     | 0.48              |
| 1:CA:174:C:O2'     | 1:CA:175:C:H5'     | 2.13                     | 0.48              |
| 1:CA:509:A:H2'     | 1:CA:509:A:N3      | 2.27                     | 0.48              |
| 1:CA:779:C:H2'     | 1:CA:780:A:O4'     | 2.14                     | 0.48              |
| 2:CB:187:LEU:HD22  | 2:CB:201:ILE:O     | 2.14                     | 0.48              |
| 3:CC:78:GLY:HA3    | 3:CC:83:ARG:HB3    | 1.96                     | 0.48              |
| 5:CE:28:PHE:CD2    | 5:CE:51:VAL:HG22   | 2.48                     | 0.48              |
| 12:CL:41:ARG:HG2   | 12:CL:42:THR:N     | 2.23                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1047:G:H5''   | 14:CN:4:LYS:HD3    | 1.96                     | 0.48              |
| 24:CY:13:ARG:NH1   | 24:CY:277:VAL:HG23 | 2.27                     | 0.48              |
| 24:CY:208:GLN:O    | 24:CY:209:ALA:O    | 2.31                     | 0.48              |
| 24:CY:137:ASN:ND2  | 24:CY:263:ALA:CB   | 2.76                     | 0.48              |
| 24:CY:264:LEU:HD22 | 24:CY:265:LYS:HZ3  | 1.79                     | 0.48              |
| 24:CY:312:LEU:HD11 | 24:CY:401:SER:OG   | 2.13                     | 0.48              |
| 24:CY:92:ILE:CB    | 24:CY:405:PRO:HG2  | 2.43                     | 0.48              |
| 24:CY:610:VAL:O    | 24:CY:610:VAL:HG23 | 2.12                     | 0.48              |
| 26:D1:67:ILE:N     | 26:D1:68:PRO:CD    | 2.71                     | 0.48              |
| 31:D6:8:LYS:HZ1    | 35:DA:2285:C:H5    | 1.53                     | 0.48              |
| 33:D8:50:LEU:O     | 33:D8:52:LYS:N     | 2.34                     | 0.48              |
| 35:DA:112:U:C2'    | 35:DA:113:G:H5'    | 2.44                     | 0.48              |
| 35:DA:1141:U:H1'   | 35:DA:1142(A):A:C2 | 2.48                     | 0.48              |
| 35:DA:1491:G:H21   | 35:DA:1492:G:H1'   | 1.77                     | 0.48              |
| 35:DA:1721:G:O6    | 35:DA:1739:U:H5'   | 2.14                     | 0.48              |
| 35:DA:1788:C:H2'   | 35:DA:1789:A:H8    | 1.77                     | 0.48              |
| 35:DA:230:U:O2'    | 35:DA:231:C:H5'    | 2.12                     | 0.48              |
| 35:DA:295:G:O2'    | 35:DA:296:C:H5'    | 2.13                     | 0.48              |
| 35:DA:363(F):A:H1' | 35:DA:364:C:H5     | 1.78                     | 0.48              |
| 35:DA:557:U:H2'    | 35:DA:558:G:H8     | 1.77                     | 0.48              |
| 31:D6:42:TRP:CH2   | 35:DA:643:A:N7     | 2.81                     | 0.48              |
| 32:D7:11:LYS:HE2   | 35:DA:686:G:H5''   | 1.95                     | 0.48              |
| 35:DA:729:G:OP2    | 38:DD:13:ARG:NH1   | 2.46                     | 0.48              |
| 35:DA:739:G:HO2'   | 35:DA:740:U:H6     | 1.60                     | 0.48              |
| 35:DA:755:C:H2'    | 35:DA:756:C:C6     | 2.49                     | 0.48              |
| 35:DA:760:G:C2'    | 35:DA:761:A:H5'    | 2.44                     | 0.48              |
| 35:DA:777:A:H2'    | 35:DA:778:G:H8     | 1.77                     | 0.48              |
| 35:DA:786:C:C2'    | 35:DA:787:U:H5'    | 2.43                     | 0.48              |
| 35:DA:821:A:O2'    | 35:DA:945:A:H3'    | 2.13                     | 0.48              |
| 40:DF:89:VAL:O     | 40:DF:91:GLY:N     | 2.43                     | 0.48              |
| 42:DH:83:TYR:CB    | 42:DH:134:SER:HA   | 2.38                     | 0.48              |
| 42:DH:17:VAL:HB    | 42:DH:45:VAL:HG13  | 1.95                     | 0.48              |
| 46:DN:2:LYS:HZ3    | 54:DV:12:TYR:HA    | 1.77                     | 0.48              |
| 47:DO:108:GLU:N    | 47:DO:108:GLU:OE2  | 2.44                     | 0.48              |
| 48:DP:64:LYS:O     | 48:DP:66:GLY:N     | 2.40                     | 0.48              |
| 55:DW:6:ILE:HG13   | 55:DW:104:THR:HG23 | 1.95                     | 0.48              |
| 58:DZ:17:ALA:HA    | 58:DZ:20:ARG:HD3   | 1.95                     | 0.48              |
| 58:DZ:55:HIS:CE1   | 58:DZ:135:GLU:OE2  | 2.65                     | 0.48              |
| 1:AA:1030:C:N4     | 1:AA:1032:G:C2     | 2.82                     | 0.48              |
| 1:AA:1124:G:C5'    | 10:AJ:35:SER:HB2   | 2.43                     | 0.48              |
| 1:AA:603:U:H2'     | 1:AA:604:G:H8      | 1.77                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:779:C:H2'     | 1:AA:780:A:O4'     | 2.13                     | 0.48              |
| 1:AA:819:A:H4'     | 1:AA:820:U:OP2     | 2.13                     | 0.48              |
| 1:AA:858:G:O2'     | 1:AA:859:A:H5''    | 2.13                     | 0.48              |
| 2:AB:44:LEU:CD1    | 2:AB:44:LEU:H      | 2.12                     | 0.48              |
| 6:AF:33:TYR:O      | 6:AF:34:GLY:C      | 2.52                     | 0.48              |
| 1:AA:878:G:H5'     | 8:AH:89:PRO:HG2    | 1.95                     | 0.48              |
| 9:AI:56:LEU:HD23   | 9:AI:56:LEU:C      | 2.33                     | 0.48              |
| 9:AI:26:VAL:CG2    | 9:AI:61:ALA:HB3    | 2.39                     | 0.48              |
| 12:AL:27:LEU:CG    | 12:AL:62:SER:HB2   | 2.43                     | 0.48              |
| 20:AT:33:ILE:HD13  | 20:AT:63:ILE:HA    | 1.94                     | 0.48              |
| 24:AY:646:PHE:O    | 24:AY:647:VAL:HG13 | 2.13                     | 0.48              |
| 31:B6:10:LEU:HB3   | 33:B8:34:TRP:HD1   | 1.78                     | 0.48              |
| 31:B6:15:GLU:O     | 31:B6:16:CYS:O     | 2.30                     | 0.48              |
| 35:BA:1210:A:H5''  | 35:BA:1212:G:O4'   | 2.13                     | 0.48              |
| 35:BA:1275:A:C4    | 50:BR:16:HIS:ND1   | 2.81                     | 0.48              |
| 35:BA:1285:G:C2'   | 35:BA:1286:A:H5'   | 2.38                     | 0.48              |
| 35:BA:1719:G:O2'   | 35:BA:1720:U:H5'   | 2.13                     | 0.48              |
| 35:BA:177:G:H3'    | 35:BA:178:G:H8     | 1.78                     | 0.48              |
| 35:BA:1899:G:N2    | 35:BA:1902:C:C4    | 2.80                     | 0.48              |
| 35:BA:2320:A:C2    | 35:BA:2333:A:C8    | 3.01                     | 0.48              |
| 35:BA:2352:A:H2'   | 35:BA:2353:G:H5'   | 1.95                     | 0.48              |
| 35:BA:278:A:C2     | 35:BA:279:C:C2     | 3.01                     | 0.48              |
| 35:BA:322:A:P      | 40:BF:169:ASN:HD22 | 2.37                     | 0.48              |
| 35:BA:453:C:H4'    | 35:BA:472:A:N6     | 2.29                     | 0.48              |
| 35:BA:588:U:H2'    | 35:BA:589:C:C6     | 2.47                     | 0.48              |
| 37:BC:90:ALA:HA    | 37:BC:155:ARG:HH12 | 1.77                     | 0.48              |
| 38:BD:165:ILE:HD13 | 38:BD:175:LEU:HD21 | 1.95                     | 0.48              |
| 40:BF:174:VAL:HG21 | 40:BF:189:THR:CG2  | 2.42                     | 0.48              |
| 40:BF:206:ILE:HG22 | 40:BF:207:GLY:H    | 1.78                     | 0.48              |
| 41:BG:133:LEU:CD1  | 41:BG:157:ILE:HB   | 2.43                     | 0.48              |
| 41:BG:153:ARG:HB3  | 41:BG:153:ARG:HH11 | 1.79                     | 0.48              |
| 42:BH:144:VAL:HA   | 42:BH:147:ASN:HB2  | 1.94                     | 0.48              |
| 42:BH:41:MET:SD    | 42:BH:53:GLU:N     | 2.86                     | 0.48              |
| 35:BA:1081:U:H4'   | 44:BK:117:THR:CG2  | 2.44                     | 0.48              |
| 46:BN:15:LEU:HD23  | 46:BN:53:VAL:HB    | 1.94                     | 0.48              |
| 35:BA:636:G:H2'    | 48:BP:115:LEU:HD12 | 1.95                     | 0.48              |
| 50:BR:38:VAL:CB    | 50:BR:39:PRO:HD3   | 2.36                     | 0.48              |
| 53:BU:10:ARG:O     | 53:BU:12:ARG:N     | 2.47                     | 0.48              |
| 58:BZ:129:SER:C    | 58:BZ:131:ARG:N    | 2.64                     | 0.48              |
| 58:BZ:17:ALA:HA    | 58:BZ:20:ARG:HG2   | 1.94                     | 0.48              |
| 58:BZ:29:TYR:HA    | 58:BZ:33:LEU:O     | 2.13                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1152:A:OP1    | 10:CJ:68:HIS:CD2   | 2.65                     | 0.48              |
| 1:CA:505:G:H5'     | 1:CA:534:U:H2'     | 1.96                     | 0.48              |
| 1:CA:554:C:H2'     | 1:CA:555:C:C6      | 2.49                     | 0.48              |
| 1:CA:624:C:H4'     | 16:CP:10:GLY:C     | 2.33                     | 0.48              |
| 3:CC:69:HIS:HA     | 3:CC:104:GLN:HB2   | 1.95                     | 0.48              |
| 4:CD:159:ARG:O     | 4:CD:163:GLU:N     | 2.46                     | 0.48              |
| 10:CJ:94:VAL:CG1   | 10:CJ:95:GLU:N     | 2.76                     | 0.48              |
| 11:CK:30:VAL:HG21  | 11:CK:65:ALA:HA    | 1.94                     | 0.48              |
| 12:CL:51:ALA:O     | 12:CL:52:LEU:HD23  | 2.13                     | 0.48              |
| 12:CL:8:ASN:O      | 12:CL:12:ARG:HG3   | 2.13                     | 0.48              |
| 18:CR:56:THR:CB    | 18:CR:58:LEU:HD13  | 2.35                     | 0.48              |
| 24:CY:74:TRP:CD1   | 24:CY:273:LEU:HB3  | 2.49                     | 0.48              |
| 24:CY:315:LYS:NZ   | 24:CY:317:MET:HG2  | 2.27                     | 0.48              |
| 24:CY:519:ARG:NH1  | 24:CY:678:GLU:N    | 2.54                     | 0.48              |
| 24:CY:580:MET:O    | 24:CY:580:MET:HG2  | 2.12                     | 0.48              |
| 29:D4:2:LYS:HB2    | 36:DB:40:U:C4      | 2.47                     | 0.48              |
| 35:DA:1081:U:H4'   | 44:DK:117:THR:CG2  | 2.42                     | 0.48              |
| 35:DA:1799:G:H5'   | 35:DA:1819:A:N6    | 2.28                     | 0.48              |
| 35:DA:1930:G:C2'   | 35:DA:1931:U:OP2   | 2.61                     | 0.48              |
| 35:DA:2137:C:H2'   | 35:DA:2138:C:C6    | 2.49                     | 0.48              |
| 35:DA:2208:A:H1'   | 35:DA:2219:G:C4    | 2.48                     | 0.48              |
| 35:DA:2229:C:O2'   | 35:DA:2230:G:H5'   | 2.13                     | 0.48              |
| 35:DA:229:A:OP1    | 35:DA:229:A:H8     | 1.95                     | 0.48              |
| 35:DA:2309:A:C2'   | 35:DA:2310:A:H5''  | 2.43                     | 0.48              |
| 35:DA:25:U:H2'     | 35:DA:26:G:O4'     | 2.13                     | 0.48              |
| 35:DA:465:G:H2'    | 35:DA:466:A:C8     | 2.49                     | 0.48              |
| 35:DA:537:C:O5'    | 35:DA:537:C:H6     | 1.96                     | 0.48              |
| 31:D6:42:TRP:NE1   | 35:DA:643:A:OP1    | 2.46                     | 0.48              |
| 35:DA:900:A:C8     | 35:DA:900:A:H5'    | 2.44                     | 0.48              |
| 37:DC:74:ARG:N     | 37:DC:112:ASP:HB2  | 2.27                     | 0.48              |
| 37:DC:65:LEU:HD11  | 37:DC:162:ILE:HD13 | 1.96                     | 0.48              |
| 38:DD:39:LYS:HB2   | 38:DD:62:TYR:HB2   | 1.95                     | 0.48              |
| 40:DF:170:LEU:HD22 | 40:DF:170:LEU:N    | 2.28                     | 0.48              |
| 40:DF:41:LEU:HD23  | 40:DF:44:ARG:HE    | 1.79                     | 0.48              |
| 36:DB:57:A:C4      | 41:DG:29:TRP:HB2   | 2.49                     | 0.48              |
| 44:DK:121:GLU:O    | 44:DK:125:ARG:HG3  | 2.14                     | 0.48              |
| 46:DN:3:THR:CG2    | 46:DN:5:VAL:HG23   | 2.42                     | 0.48              |
| 46:DN:9:VAL:HG12   | 46:DN:10:GLU:H     | 1.77                     | 0.48              |
| 35:DA:1666:G:O3'   | 47:DO:6:THR:HG23   | 2.13                     | 0.48              |
| 48:DP:101:VAL:HG12 | 48:DP:106:LEU:CB   | 2.41                     | 0.48              |
| 49:DQ:134:ARG:HG3  | 49:DQ:134:ARG:HH11 | 1.77                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:DR:21:TYR:OH    | 50:DR:43:GLU:HG2   | 2.13                     | 0.48              |
| 52:DT:108:ARG:HB2  | 52:DT:108:ARG:HH11 | 1.78                     | 0.48              |
| 56:DX:70:LEU:C     | 56:DX:70:LEU:HD23  | 2.33                     | 0.48              |
| 58:DZ:16:SER:OG    | 58:DZ:17:ALA:N     | 2.46                     | 0.48              |
| 1:AA:1118:C:H1'    | 1:AA:1179:A:C4     | 2.49                     | 0.48              |
| 1:AA:1286:A:H2'    | 1:AA:1287:A:H4'    | 1.95                     | 0.48              |
| 1:AA:948:C:H2'     | 1:AA:949:A:H8      | 1.78                     | 0.48              |
| 3:AC:115:LEU:O     | 3:AC:116:VAL:C     | 2.51                     | 0.48              |
| 6:AF:50:TYR:CE1    | 18:AR:77:GLY:HA2   | 2.47                     | 0.48              |
| 7:AG:5:ARG:N       | 7:AG:5:ARG:HD2     | 2.28                     | 0.48              |
| 1:AA:1345:U:OP1    | 9:AI:120:ARG:NH1   | 2.46                     | 0.48              |
| 1:AA:1147:C:O2'    | 9:AI:16:ARG:HD2    | 2.14                     | 0.48              |
| 9:AI:5:TYR:HD2     | 9:AI:17:VAL:O      | 1.96                     | 0.48              |
| 10:AJ:63:PHE:HA    | 14:AN:59:ALA:CB    | 2.43                     | 0.48              |
| 10:AJ:78:ASN:C     | 10:AJ:79:ARG:NH1   | 2.67                     | 0.48              |
| 11:AK:29:ILE:HB    | 11:AK:44:SER:CB    | 2.44                     | 0.48              |
| 13:AM:116:THR:CG2  | 13:AM:117:VAL:N    | 2.76                     | 0.48              |
| 14:AN:60:SER:O     | 14:AN:61:TRP:HB3   | 2.14                     | 0.48              |
| 15:AO:55:GLY:HA2   | 15:AO:58:MET:CE    | 2.41                     | 0.48              |
| 18:AR:88:LYS:C     | 18:AR:88:LYS:HD3   | 2.34                     | 0.48              |
| 19:AS:51:VAL:HG22  | 19:AS:71:LEU:HD13  | 1.95                     | 0.48              |
| 21:AU:10:ARG:O     | 21:AU:13:ILE:N     | 2.46                     | 0.48              |
| 24:AY:518:PRO:O    | 24:AY:520:GLY:N    | 2.46                     | 0.48              |
| 24:AY:549:ALA:HB2  | 24:AY:587:SER:OG   | 2.13                     | 0.48              |
| 61:AY:702:FUA:C1   | 61:AY:702:FUA:O1   | 2.60                     | 0.48              |
| 31:B6:11:LEU:HD23  | 31:B6:51:GLU:CG    | 2.44                     | 0.48              |
| 35:BA:1972:A:H2'   | 35:BA:1973:G:C8    | 2.47                     | 0.48              |
| 35:BA:2389:G:C5'   | 35:BA:2390:U:H5'   | 2.41                     | 0.48              |
| 35:BA:2539:C:O2    | 35:BA:2539:C:H2'   | 2.12                     | 0.48              |
| 35:BA:2716:U:O2'   | 35:BA:2717:G:H5'   | 2.13                     | 0.48              |
| 35:BA:654(O):G:H2' | 35:BA:654(P):C:C6  | 2.48                     | 0.48              |
| 35:BA:654(P):C:H2' | 35:BA:654(Q):C:C5' | 2.44                     | 0.48              |
| 36:BB:20:C:C2'     | 36:BB:21:G:C5'     | 2.91                     | 0.48              |
| 40:BF:123:LEU:HD12 | 40:BF:124:LEU:H    | 1.76                     | 0.48              |
| 40:BF:18:ARG:CZ    | 40:BF:199:TRP:CZ3  | 2.97                     | 0.48              |
| 41:BG:34:LEU:HD13  | 41:BG:99:MET:HE2   | 1.95                     | 0.48              |
| 48:BP:85:LEU:HA    | 48:BP:88:LEU:HB3   | 1.96                     | 0.48              |
| 49:BQ:60:ARG:CZ    | 49:BQ:60:ARG:HB2   | 2.43                     | 0.48              |
| 51:BS:58:LEU:CD1   | 51:BS:59:LYS:H     | 2.26                     | 0.48              |
| 52:BT:75:ILE:N     | 52:BT:75:ILE:CD1   | 2.76                     | 0.48              |
| 53:BU:52:ARG:O     | 53:BU:55:ARG:HG2   | 2.13                     | 0.48              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:BZ:10:ARG:NH2   | 58:BZ:26:GLY:O     | 2.45                     | 0.48              |
| 49:BQ:62:GLY:CA    | 58:BZ:116:VAL:HG21 | 2.43                     | 0.48              |
| 1:CA:1343:G:H1'    | 9:CI:121:ARG:NH1   | 2.28                     | 0.48              |
| 1:CA:1388:C:H2'    | 1:CA:1389:C:H6     | 1.79                     | 0.48              |
| 1:CA:1459:C:H2'    | 1:CA:1460:A:H8     | 1.75                     | 0.48              |
| 1:CA:404:U:H2'     | 1:CA:405:U:C6      | 2.48                     | 0.48              |
| 1:CA:703:G:C2'     | 1:CA:704:A:OP2     | 2.61                     | 0.48              |
| 1:CA:78:G:H1       | 1:CA:91:C:N4       | 2.11                     | 0.48              |
| 5:CE:68:GLU:O      | 5:CE:68:GLU:HG3    | 2.11                     | 0.48              |
| 10:CJ:4:ILE:HB     | 10:CJ:74:ILE:HG13  | 1.95                     | 0.48              |
| 24:CY:164:MET:HG3  | 24:CY:259:PHE:CZ   | 2.49                     | 0.48              |
| 24:CY:539:ILE:O    | 24:CY:540:PRO:C    | 2.52                     | 0.48              |
| 33:D8:4:MET:CE     | 33:D8:61:LEU:HD22  | 2.44                     | 0.48              |
| 33:D8:55:ALA:O     | 33:D8:59:LYS:HE2   | 2.12                     | 0.48              |
| 35:DA:1141:U:OP2   | 46:DN:63:THR:OG1   | 2.22                     | 0.48              |
| 35:DA:1169:G:C2    | 35:DA:1181:C:N3    | 2.81                     | 0.48              |
| 35:DA:2135:A:H2'   | 35:DA:2136:C:O4'   | 2.13                     | 0.48              |
| 35:DA:271(Z):C:H1' | 35:DA:272(C):G:H1' | 1.96                     | 0.48              |
| 35:DA:445:C:O2'    | 35:DA:446:G:H5'    | 2.13                     | 0.48              |
| 35:DA:453:C:H4'    | 35:DA:472:A:N6     | 2.28                     | 0.48              |
| 36:DB:15:A:C3'     | 36:DB:16:G:H5'     | 2.42                     | 0.48              |
| 37:DC:196:ALA:O    | 37:DC:199:ALA:HB3  | 2.13                     | 0.48              |
| 38:DD:96:HIS:CE1   | 38:DD:102:LYS:HE2  | 2.48                     | 0.48              |
| 38:DD:227:ASN:HB3  | 38:DD:228:PRO:HD2  | 1.94                     | 0.48              |
| 38:DD:35:LYS:NZ    | 38:DD:35:LYS:HB3   | 2.28                     | 0.48              |
| 39:DE:170:LEU:H    | 39:DE:170:LEU:CD1  | 2.25                     | 0.48              |
| 39:DE:51:PHE:CD1   | 39:DE:52:LEU:HD12  | 2.48                     | 0.48              |
| 39:DE:76:ARG:O     | 39:DE:77:ILE:O     | 2.32                     | 0.48              |
| 41:DG:181:ARG:HH11 | 41:DG:181:ARG:CG   | 2.26                     | 0.48              |
| 44:DK:88:ALA:O     | 44:DK:90:LYS:N     | 2.44                     | 0.48              |
| 47:DO:9:GLU:O      | 47:DO:83:ALA:HA    | 2.13                     | 0.48              |
| 50:DR:12:ARG:HB3   | 50:DR:16:HIS:HD2   | 1.79                     | 0.48              |
| 53:DU:47:TYR:O     | 53:DU:51:LYS:HG2   | 2.13                     | 0.48              |
| 53:DU:82:GLY:O     | 53:DU:84:LYS:N     | 2.46                     | 0.48              |
| 55:DW:36:LEU:HD12  | 55:DW:48:ALA:HA    | 1.96                     | 0.48              |
| 57:DY:29:GLU:N     | 57:DY:29:GLU:OE1   | 2.46                     | 0.48              |
| 1:AA:1122:U:O2'    | 1:AA:1123:A:H5'    | 2.13                     | 0.48              |
| 1:AA:1525:G:O2'    | 1:AA:1526:G:H5'    | 2.13                     | 0.48              |
| 1:AA:155:C:H2'     | 1:AA:156:G:H8      | 1.78                     | 0.48              |
| 1:AA:60:A:C5'      | 1:AA:331:G:H22     | 2.26                     | 0.48              |
| 1:AA:538:G:OP2     | 12:AL:115:LYS:HG3  | 2.13                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:771:G:H2'     | 1:AA:772:U:C6      | 2.48                     | 0.48              |
| 1:AA:963:G:H21     | 10:AJ:55:LYS:CD    | 2.27                     | 0.48              |
| 1:AA:967:C:H2'     | 1:AA:968:A:C8      | 2.48                     | 0.48              |
| 3:AC:155:GLY:O     | 3:AC:156:ARG:CB    | 2.61                     | 0.48              |
| 7:AG:105:VAL:O     | 7:AG:108:ALA:HB3   | 2.13                     | 0.48              |
| 1:AA:1123:A:O3'    | 10:AJ:36:GLY:HA3   | 2.14                     | 0.48              |
| 10:AJ:56:HIS:O     | 10:AJ:58:ASP:N     | 2.46                     | 0.48              |
| 13:AM:97:PRO:HA    | 13:AM:110:ARG:CD   | 2.35                     | 0.48              |
| 24:AY:250:THR:O    | 24:AY:253:LEU:N    | 2.35                     | 0.48              |
| 27:B2:17:SER:HB2   | 27:B2:18:PRO:HD2   | 1.96                     | 0.48              |
| 27:B2:39:ALA:HA    | 27:B2:45:SER:HB3   | 1.95                     | 0.48              |
| 35:BA:1362:C:H2'   | 35:BA:1363:C:H6    | 1.78                     | 0.48              |
| 35:BA:1630:G:C2    | 35:BA:1637:A:C2    | 3.01                     | 0.48              |
| 35:BA:1748:G:C8    | 35:BA:1748:G:H5'   | 2.40                     | 0.48              |
| 35:BA:1799:G:H5'   | 35:BA:1819:A:N6    | 2.29                     | 0.48              |
| 35:BA:2050:C:H2'   | 35:BA:2051:A:O4'   | 2.13                     | 0.48              |
| 35:BA:2328:A:H2'   | 35:BA:2329:G:C8    | 2.48                     | 0.48              |
| 35:BA:2464:C:O2'   | 35:BA:2465:C:O5'   | 2.32                     | 0.48              |
| 35:BA:325:G:O2'    | 35:BA:326:G:H5'    | 2.13                     | 0.48              |
| 35:BA:900:A:H5'    | 35:BA:900:A:C8     | 2.44                     | 0.48              |
| 36:BB:81:G:C2      | 36:BB:82:G:N7      | 2.82                     | 0.48              |
| 38:BD:35:LYS:HD2   | 38:BD:36:PRO:HA    | 1.93                     | 0.48              |
| 39:BE:170:LEU:H    | 39:BE:170:LEU:CD1  | 2.24                     | 0.48              |
| 41:BG:7:LEU:HB3    | 41:BG:100:TRP:CE3  | 2.48                     | 0.48              |
| 47:BO:88:ASN:C     | 47:BO:90:GLN:H     | 2.17                     | 0.48              |
| 48:BP:67:MET:C     | 48:BP:68:GLN:HG3   | 2.33                     | 0.48              |
| 48:BP:77:ARG:HB2   | 48:BP:78:PRO:CD    | 2.40                     | 0.48              |
| 50:BR:100:LEU:N    | 50:BR:100:LEU:HD13 | 2.28                     | 0.48              |
| 51:BS:12:PHE:CD1   | 51:BS:12:PHE:C     | 2.87                     | 0.48              |
| 52:BT:57:PHE:O     | 52:BT:58:ASN:C     | 2.50                     | 0.48              |
| 53:BU:112:ARG:CG   | 53:BU:112:ARG:HH11 | 2.26                     | 0.48              |
| 54:BV:19:LYS:HE2   | 54:BV:19:LYS:HA    | 1.96                     | 0.48              |
| 55:BW:6:ILE:HG13   | 55:BW:104:THR:HG23 | 1.95                     | 0.48              |
| 58:BZ:5:LEU:HB3    | 58:BZ:59:LEU:HD23  | 1.95                     | 0.48              |
| 1:CA:1030(C):G:H2' | 1:CA:1030(D):A:C8  | 2.47                     | 0.48              |
| 1:CA:1325:C:C2     | 1:CA:1326:C:C5     | 3.01                     | 0.48              |
| 1:CA:177:C:H2'     | 1:CA:178:C:H6      | 1.79                     | 0.48              |
| 1:CA:967:C:H2'     | 1:CA:968:A:C8      | 2.49                     | 0.48              |
| 2:CB:51:LEU:CD2    | 2:CB:201:ILE:HG23  | 2.43                     | 0.48              |
| 3:CC:5:ILE:O       | 3:CC:5:ILE:HD13    | 2.14                     | 0.48              |
| 4:CD:8:VAL:C       | 4:CD:10:ARG:H      | 2.14                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:CF:42:GLU:C     | 6:CF:44:GLY:N     | 2.67                     | 0.48              |
| 12:CL:27:LEU:CG   | 12:CL:62:SER:HB2  | 2.43                     | 0.48              |
| 12:CL:6:THR:H     | 12:CL:9:GLN:NE2   | 2.12                     | 0.48              |
| 13:CM:74:VAL:CA   | 13:CM:77:ASN:HD22 | 2.27                     | 0.48              |
| 1:CA:1316:G:H4'   | 14:CN:18:VAL:HG12 | 1.95                     | 0.48              |
| 14:CN:60:SER:O    | 14:CN:61:TRP:HB3  | 2.14                     | 0.48              |
| 15:CO:43:LEU:CD1  | 15:CO:56:LEU:HD22 | 2.44                     | 0.48              |
| 16:CP:67:THR:HB   | 16:CP:70:ALA:HB2  | 1.96                     | 0.48              |
| 18:CR:87:ARG:CB   | 18:CR:87:ARG:HH11 | 2.26                     | 0.48              |
| 20:CT:50:GLU:HG3  | 20:CT:51:GLU:H    | 1.77                     | 0.48              |
| 24:CY:453:GLY:HA3 | 24:CY:459:LEU:CD2 | 2.43                     | 0.48              |
| 24:CY:538:TYR:CD1 | 24:CY:579:GLU:HA  | 2.49                     | 0.48              |
| 24:CY:652:MET:HE2 | 24:CY:655:TYR:HB2 | 1.96                     | 0.48              |
| 24:CY:73:PHE:HZ   | 24:CY:78:ARG:NH2  | 2.11                     | 0.48              |
| 26:D1:6:GLU:OE1   | 26:D1:61:ARG:N    | 2.46                     | 0.48              |
| 28:D3:28:LEU:CD2  | 28:D3:35:ARG:HD2  | 2.44                     | 0.48              |
| 28:D3:46:ASN:O    | 28:D3:49:LYS:N    | 2.47                     | 0.48              |
| 30:D5:56:LYS:O    | 30:D5:57:VAL:O    | 2.31                     | 0.48              |
| 33:D8:4:MET:HE1   | 33:D8:61:LEU:HD22 | 1.95                     | 0.48              |
| 35:DA:1045:A:N3   | 35:DA:1047:G:N2   | 2.61                     | 0.48              |
| 35:DA:1052:C:O2'  | 35:DA:1053:C:O5'  | 2.32                     | 0.48              |
| 35:DA:1100:C:O2   | 35:DA:1100:C:H2'  | 2.14                     | 0.48              |
| 35:DA:1270:C:H5'' | 35:DA:1271:G:O5'  | 2.14                     | 0.48              |
| 35:DA:350:U:H2'   | 35:DA:351:G:O4'   | 2.14                     | 0.48              |
| 35:DA:552:G:O2'   | 35:DA:553:G:H5'   | 2.13                     | 0.48              |
| 35:DA:733:G:C6    | 35:DA:761:A:N7    | 2.81                     | 0.48              |
| 35:DA:781:A:H2'   | 35:DA:1777:U:O2'  | 2.13                     | 0.48              |
| 36:DB:54:G:H2'    | 36:DB:55:U:H6     | 1.78                     | 0.48              |
| 38:DD:213:ARG:C   | 38:DD:215:LEU:N   | 2.66                     | 0.48              |
| 40:DF:9:ILE:HG12  | 40:DF:14:PRO:HA   | 1.94                     | 0.48              |
| 40:DF:150:GLY:HA2 | 40:DF:172:TRP:CE3 | 2.48                     | 0.48              |
| 40:DF:179:GLU:C   | 40:DF:181:LEU:H   | 2.16                     | 0.48              |
| 41:DG:51:ARG:NH1  | 41:DG:53:LEU:HD21 | 2.28                     | 0.48              |
| 42:DH:144:VAL:HA  | 42:DH:147:ASN:HB2 | 1.95                     | 0.48              |
| 48:DP:46:LYS:HG2  | 48:DP:52:GLU:HG2  | 1.96                     | 0.48              |
| 35:DA:245:G:H5'   | 48:DP:73:GLY:HA2  | 1.94                     | 0.48              |
| 49:DQ:37:LEU:HD12 | 49:DQ:128:LYS:HB3 | 1.96                     | 0.48              |
| 49:DQ:12:GLN:HE21 | 49:DQ:73:PRO:CD   | 2.22                     | 0.48              |
| 50:DR:51:LEU:HD12 | 50:DR:51:LEU:H    | 1.78                     | 0.48              |
| 52:DT:28:VAL:HG13 | 52:DT:46:GLU:CA   | 2.41                     | 0.48              |
| 54:DV:2:PHE:O     | 54:DV:3:ALA:CB    | 2.62                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:487:C:H1'    | 55:DW:53:SER:HA    | 1.96                     | 0.48              |
| 58:DZ:109:ALA:O    | 58:DZ:111:VAL:N    | 2.47                     | 0.48              |
| 1:AA:424:G:O2'     | 1:AA:425:G:H5'     | 2.13                     | 0.48              |
| 1:AA:542:G:H5'     | 4:AD:41:GLY:HA2    | 1.96                     | 0.48              |
| 3:AC:84:ILE:O      | 3:AC:84:ILE:HG12   | 2.14                     | 0.48              |
| 4:AD:23:GLY:HA3    | 4:AD:112:VAL:HG22  | 1.95                     | 0.48              |
| 4:AD:43:HIS:O      | 4:AD:45:GLN:N      | 2.47                     | 0.48              |
| 1:AA:430:A:OP2     | 4:AD:8:VAL:HG22    | 2.13                     | 0.48              |
| 10:AJ:8:LEU:HB2    | 10:AJ:70:ARG:O     | 2.13                     | 0.48              |
| 12:AL:75:HIS:CD2   | 12:AL:77:LEU:HD12  | 2.47                     | 0.48              |
| 13:AM:3:ARG:HB2    | 29:B4:34:GLU:HG2   | 1.94                     | 0.48              |
| 24:AY:128:TYR:O    | 24:AY:129:LYS:CB   | 2.60                     | 0.48              |
| 24:AY:170:ARG:HH22 | 24:AY:208:GLN:HE22 | 1.62                     | 0.48              |
| 24:AY:17:ILE:N     | 24:AY:17:ILE:CD1   | 2.77                     | 0.48              |
| 24:AY:351:ARG:O    | 24:AY:351:ARG:HG3  | 2.13                     | 0.48              |
| 24:AY:416:LYS:NZ   | 24:AY:417:THR:HG23 | 2.29                     | 0.48              |
| 24:AY:512:ILE:N    | 24:AY:512:ILE:CD1  | 2.74                     | 0.48              |
| 24:AY:539:ILE:HD12 | 24:AY:567:LEU:HD21 | 1.96                     | 0.48              |
| 32:B7:27:GLY:HA2   | 32:B7:30:VAL:HG23  | 1.96                     | 0.48              |
| 33:B8:33:ASN:N     | 33:B8:33:ASN:ND2   | 2.41                     | 0.48              |
| 33:B8:50:LEU:C     | 33:B8:53:PRO:CD    | 2.82                     | 0.48              |
| 35:BA:1141:U:H1'   | 35:BA:1142(A):A:C2 | 2.48                     | 0.48              |
| 35:BA:1328:G:H2'   | 35:BA:1330:C:C4    | 2.49                     | 0.48              |
| 35:BA:1472:A:O2'   | 35:BA:1473:G:H5'   | 2.13                     | 0.48              |
| 35:BA:1666:G:O3'   | 47:BO:6:THR:HG23   | 2.14                     | 0.48              |
| 35:BA:1909:C:O2'   | 35:BA:1910:G:H5'   | 2.14                     | 0.48              |
| 35:BA:2293:C:OP1   | 51:BS:92:TYR:OH    | 2.31                     | 0.48              |
| 35:BA:2585:U:HO2'  | 35:BA:2586:C:H5'   | 1.75                     | 0.48              |
| 35:BA:640:C:C4     | 35:BA:641:C:N4     | 2.82                     | 0.48              |
| 35:BA:654(S):G:C5  | 35:BA:654(T):C:H1' | 2.48                     | 0.48              |
| 35:BA:709:U:H2'    | 35:BA:710:G:H8     | 1.77                     | 0.48              |
| 35:BA:769:G:H5'    | 35:BA:1379:A:N6    | 2.28                     | 0.48              |
| 35:BA:849:A:C8     | 35:BA:850:C:C5     | 3.02                     | 0.48              |
| 35:BA:958:U:C3'    | 35:BA:958:U:C6     | 2.96                     | 0.48              |
| 36:BB:91:C:H5'     | 49:BQ:17:LEU:O     | 2.13                     | 0.48              |
| 37:BC:115:VAL:CG1  | 37:BC:145:THR:HG23 | 2.42                     | 0.48              |
| 38:BD:91:ARG:O     | 38:BD:107:ALA:HB3  | 2.14                     | 0.48              |
| 38:BD:26:LYS:N     | 38:BD:26:LYS:HE2   | 2.27                     | 0.48              |
| 39:BE:108:SER:O    | 39:BE:162:ALA:HA   | 2.14                     | 0.48              |
| 39:BE:177:PRO:HG2  | 39:BE:178:GLU:H    | 1.78                     | 0.48              |
| 41:BG:53:LEU:HD22  | 41:BG:53:LEU:N     | 2.29                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 41:BG:82:LEU:HD21  | 41:BG:87:PRO:HG3    | 1.95                     | 0.48              |
| 48:BP:112:LEU:N    | 48:BP:128:HIS:HD2   | 2.12                     | 0.48              |
| 48:BP:17:LYS:HG2   | 48:BP:17:LYS:O      | 2.13                     | 0.48              |
| 49:BQ:68:ILE:HG23  | 49:BQ:103:MET:HA    | 1.94                     | 0.48              |
| 49:BQ:17:LEU:C     | 49:BQ:18:LYS:HD2    | 2.34                     | 0.48              |
| 51:BS:106:ARG:O    | 51:BS:107:GLU:HB2   | 2.13                     | 0.48              |
| 51:BS:70:GLY:C     | 51:BS:72:ALA:N      | 2.67                     | 0.48              |
| 53:BU:113:ALA:O    | 53:BU:115:ALA:N     | 2.46                     | 0.48              |
| 53:BU:49:HIS:O     | 53:BU:52:ARG:HB2    | 2.14                     | 0.48              |
| 53:BU:95:LEU:O     | 53:BU:98:LEU:HG     | 2.13                     | 0.48              |
| 55:BW:24:ILE:HG21  | 55:BW:36:LEU:HD21   | 1.96                     | 0.48              |
| 57:BY:95:LYS:HD3   | 57:BY:100:ALA:CB    | 2.44                     | 0.48              |
| 57:BY:31:LEU:HD23  | 57:BY:36:ALA:H      | 1.79                     | 0.48              |
| 58:BZ:130:PRO:O    | 58:BZ:133:ILE:CD1   | 2.61                     | 0.48              |
| 58:BZ:71:VAL:CG1   | 58:BZ:74:VAL:HG23   | 2.43                     | 0.48              |
| 1:CA:1010:G:N1     | 1:CA:1020:U:H1'     | 2.28                     | 0.48              |
| 1:CA:1161:C:O2'    | 1:CA:1162:C:H5'     | 2.13                     | 0.48              |
| 1:CA:1497:G:H2'    | 1:CA:1498:U:H5'     | 1.95                     | 0.48              |
| 1:CA:819:A:H4'     | 1:CA:820:U:OP2      | 2.14                     | 0.48              |
| 2:CB:233:SER:CB    | 2:CB:234:PRO:HD2    | 2.44                     | 0.48              |
| 2:CB:48:MET:HA     | 2:CB:51:LEU:HD12    | 1.95                     | 0.48              |
| 8:CH:85:ARG:HH12   | 8:CH:134:ILE:HG23   | 1.79                     | 0.48              |
| 11:CK:15:ALA:HA    | 11:CK:76:GLY:O      | 2.12                     | 0.48              |
| 12:CL:86:ARG:O     | 12:CL:86:ARG:HG2    | 2.14                     | 0.48              |
| 1:CA:255:G:O3'     | 17:CQ:17:LYS:HD2    | 2.13                     | 0.48              |
| 19:CS:5:LEU:HD12   | 19:CS:8:GLY:C       | 2.34                     | 0.48              |
| 22:CW:11:A:O2'     | 22:CW:12:G:H5'      | 2.14                     | 0.48              |
| 25:D0:5:LYS:HB3    | 25:D0:5:LYS:NZ      | 2.28                     | 0.48              |
| 27:D2:52:ASP:O     | 27:D2:53:LEU:C      | 2.52                     | 0.48              |
| 27:D2:7:ARG:HG3    | 27:D2:7:ARG:HH11    | 1.79                     | 0.48              |
| 28:D3:44:ARG:O     | 28:D3:48:GLU:HG2    | 2.14                     | 0.48              |
| 33:D8:51:ALA:HA    | 33:D8:54:GLU:CD     | 2.34                     | 0.48              |
| 27:D2:65:ASN:HD21  | 35:DA:112:U:C5'     | 2.27                     | 0.48              |
| 35:DA:1186:G:C2'   | 35:DA:1187:G:H5'    | 2.43                     | 0.48              |
| 35:DA:578:A:H5'    | 35:DA:1254:A:OP1    | 2.14                     | 0.48              |
| 35:DA:1909:C:O2'   | 35:DA:1910:G:H5'    | 2.13                     | 0.48              |
| 35:DA:2097:C:O2'   | 35:DA:2098:U:H5'    | 2.13                     | 0.48              |
| 35:DA:2182:G:H2'   | 35:DA:2183:C:C6     | 2.49                     | 0.48              |
| 35:DA:2369:A:H2'   | 35:DA:2370:G:H8     | 1.79                     | 0.48              |
| 35:DA:272(G):C:C3' | 35:DA:272(H):C:H5'' | 2.44                     | 0.48              |
| 35:DA:2754:U:H2'   | 35:DA:2756:U:OP1    | 2.14                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:DE:108:SER:O    | 39:DE:162:ALA:HA   | 2.13                     | 0.48              |
| 41:DG:55:LYS:C     | 41:DG:57:ALA:H     | 2.16                     | 0.48              |
| 48:DP:106:LEU:HD11 | 48:DP:112:LEU:HD23 | 1.94                     | 0.48              |
| 48:DP:64:LYS:C     | 48:DP:66:GLY:N     | 2.66                     | 0.48              |
| 35:DA:385:C:O2     | 48:DP:71:VAL:HG21  | 2.14                     | 0.48              |
| 49:DQ:52:VAL:HG12  | 49:DQ:53:ALA:N     | 2.28                     | 0.48              |
| 50:DR:87:TYR:C     | 50:DR:89:ASP:N     | 2.65                     | 0.48              |
| 52:DT:102:ILE:HG13 | 52:DT:103:ARG:N    | 2.28                     | 0.48              |
| 52:DT:11:GLU:O     | 52:DT:13:ARG:N     | 2.37                     | 0.48              |
| 1:AA:1065:U:O2'    | 1:AA:1066:C:P      | 2.71                     | 0.48              |
| 1:AA:1239:A:C2'    | 1:AA:1298:C:N4     | 2.74                     | 0.48              |
| 1:AA:509:A:N1      | 1:AA:510:A:C2      | 2.82                     | 0.48              |
| 1:AA:703:G:C2'     | 1:AA:704:A:OP2     | 2.61                     | 0.48              |
| 1:AA:973:G:O4'     | 10:AJ:55:LYS:HE2   | 2.13                     | 0.48              |
| 1:AA:986:A:H2'     | 1:AA:987:G:C8      | 2.48                     | 0.48              |
| 2:AB:211:ILE:HG22  | 2:AB:215:LEU:HD23  | 1.95                     | 0.48              |
| 3:AC:79:ARG:HB2    | 3:AC:79:ARG:NH1    | 2.14                     | 0.48              |
| 3:AC:82:GLU:OE2    | 3:AC:82:GLU:N      | 2.47                     | 0.48              |
| 4:AD:108:LEU:HD23  | 4:AD:110:PHE:CZ    | 2.49                     | 0.48              |
| 4:AD:62:GLN:O      | 4:AD:66:ARG:HB2    | 2.13                     | 0.48              |
| 7:AG:69:VAL:HG21   | 7:AG:104:LEU:CD2   | 2.43                     | 0.48              |
| 8:AH:6:ILE:CD1     | 8:AH:6:ILE:H       | 2.27                     | 0.48              |
| 14:AN:36:PHE:CD1   | 14:AN:36:PHE:C     | 2.86                     | 0.48              |
| 20:AT:103:GLY:O    | 20:AT:104:LEU:C    | 2.52                     | 0.48              |
| 20:AT:16:HIS:O     | 20:AT:19:SER:HB3   | 2.13                     | 0.48              |
| 21:AU:3:LYS:HB3    | 21:AU:14:TRP:CD1   | 2.49                     | 0.48              |
| 22:AV:3:C:N4       | 22:AV:70:G:H1      | 2.11                     | 0.48              |
| 22:AW:15:G:H2'     | 22:AW:60:A:N1      | 2.28                     | 0.48              |
| 24:AY:451:ILE:O    | 24:AY:451:ILE:HG23 | 2.13                     | 0.48              |
| 24:AY:504:ARG:O    | 24:AY:506:GLN:N    | 2.47                     | 0.48              |
| 27:B2:24:LEU:HD23  | 27:B2:24:LEU:C     | 2.34                     | 0.48              |
| 28:B3:31:LEU:O     | 28:B3:32:GLN:CB    | 2.62                     | 0.48              |
| 30:B5:36:CYS:SG    | 30:B5:36:CYS:O     | 2.72                     | 0.48              |
| 31:B6:19:ARG:O     | 31:B6:20:ASN:C     | 2.51                     | 0.48              |
| 31:B6:7:ILE:N      | 31:B6:7:ILE:CD1    | 2.77                     | 0.48              |
| 35:BA:1598:C:H2'   | 35:BA:1599:C:C6    | 2.49                     | 0.48              |
| 35:BA:1983:C:O2'   | 35:BA:1984:G:H5'   | 2.13                     | 0.48              |
| 35:BA:2097:C:O2'   | 35:BA:2098:U:H5'   | 2.13                     | 0.48              |
| 35:BA:2691:C:H6    | 35:BA:2691:C:H5'   | 1.78                     | 0.48              |
| 35:BA:2779:U:H5'   | 35:BA:2780:G:O5'   | 2.14                     | 0.48              |
| 35:BA:303:U:H2'    | 35:BA:304:G:H8     | 1.76                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 35:BA:484:C:O2'    | 35:BA:485:C:H5'     | 2.14                     | 0.48              |
| 35:BA:544:G:H21    | 35:BA:547:A:H2'     | 1.79                     | 0.48              |
| 35:BA:667:U:H2'    | 35:BA:668:G:O4'     | 2.13                     | 0.48              |
| 32:B7:5:TRP:CH2    | 35:BA:686:G:N7      | 2.81                     | 0.48              |
| 38:BD:13:ARG:NH1   | 38:BD:16:MET:SD     | 2.87                     | 0.48              |
| 38:BD:227:ASN:O    | 38:BD:230:ASP:N     | 2.44                     | 0.48              |
| 40:BF:168:ARG:HG3  | 40:BF:175:THR:HB    | 1.95                     | 0.48              |
| 41:BG:100:TRP:O    | 41:BG:104:GLU:HB2   | 2.12                     | 0.48              |
| 42:BH:17:VAL:CG1   | 42:BH:50:VAL:HG21   | 2.38                     | 0.48              |
| 47:BO:114:ILE:H    | 47:BO:114:ILE:CD1   | 2.21                     | 0.48              |
| 48:BP:16:ARG:CB    | 48:BP:16:ARG:HH11   | 2.25                     | 0.48              |
| 48:BP:64:LYS:C     | 48:BP:66:GLY:N      | 2.67                     | 0.48              |
| 51:BS:11:LYS:N     | 51:BS:11:LYS:HD2    | 2.29                     | 0.48              |
| 52:BT:35:LYS:HZ3   | 52:BT:41:ARG:NH1    | 2.10                     | 0.48              |
| 52:BT:66:VAL:HA    | 52:BT:71:GLY:HA2    | 1.94                     | 0.48              |
| 53:BU:26:GLY:C     | 53:BU:28:ARG:N      | 2.67                     | 0.48              |
| 58:BZ:56:VAL:C     | 58:BZ:57:ILE:HD12   | 2.34                     | 0.48              |
| 1:CA:1133:G:C4     | 1:CA:1142:G:N2      | 2.81                     | 0.48              |
| 2:CB:77:ALA:O      | 2:CB:81:VAL:HG23    | 2.14                     | 0.48              |
| 3:CC:140:ARG:HG3   | 3:CC:140:ARG:HH11   | 1.78                     | 0.48              |
| 3:CC:207:VAL:HG12  | 3:CC:207:VAL:O      | 2.13                     | 0.48              |
| 9:CI:40:LEU:C      | 9:CI:42:ARG:H       | 2.16                     | 0.48              |
| 10:CJ:27:ALA:CB    | 10:CJ:85:LEU:HD11   | 2.44                     | 0.48              |
| 10:CJ:82:ILE:O     | 10:CJ:86:MET:CB     | 2.61                     | 0.48              |
| 15:CO:43:LEU:C     | 15:CO:45:VAL:H      | 2.17                     | 0.48              |
| 16:CP:28:ARG:NH1   | 16:CP:28:ARG:HG2    | 2.28                     | 0.48              |
| 24:CY:112:GLN:HG3  | 24:CY:115:GLU:HA    | 1.96                     | 0.48              |
| 24:CY:181:LEU:CD1  | 24:CY:242:LEU:HD13  | 2.44                     | 0.48              |
| 25:D0:47:PRO:HB3   | 25:D0:51:VAL:O      | 2.13                     | 0.48              |
| 27:D2:7:ARG:HG3    | 27:D2:7:ARG:NH1     | 2.27                     | 0.48              |
| 28:D3:38:GLU:HB3   | 28:D3:43:ILE:HG13   | 1.94                     | 0.48              |
| 29:D4:51:ASP:OD2   | 29:D4:52:THR:N      | 2.47                     | 0.48              |
| 31:D6:12:GLU:HB3   | 31:D6:23:THR:HG22   | 1.96                     | 0.48              |
| 35:DA:1945:G:H2'   | 35:DA:1945:G:N3     | 2.29                     | 0.48              |
| 35:DA:1956:U:C2'   | 35:DA:1957:C:H5'    | 2.44                     | 0.48              |
| 34:D9:2:LYS:HD3    | 35:DA:2526:G:N3     | 2.29                     | 0.48              |
| 35:DA:2694:G:O2'   | 35:DA:2695:C:H5'    | 2.14                     | 0.48              |
| 35:DA:272(H):C:C2' | 35:DA:272(I):U:H5'' | 2.43                     | 0.48              |
| 35:DA:614(A):U:O2' | 35:DA:614(B):G:H5'  | 2.13                     | 0.48              |
| 38:DD:125:ILE:O    | 38:DD:125:ILE:HG22  | 2.13                     | 0.48              |
| 35:DA:1675:C:O2    | 39:DE:129:HIS:HA    | 2.13                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 39:DE:16:ARG:NH1   | 39:DE:171:GLU:OE2 | 2.47                     | 0.48              |
| 35:DA:2784:C:H1'   | 39:DE:37:ARG:NH1  | 2.29                     | 0.48              |
| 40:DF:25:PRO:HB3   | 40:DF:119:ARG:HB2 | 1.96                     | 0.48              |
| 42:DH:156:ALA:C    | 42:DH:158:HIS:H   | 2.17                     | 0.48              |
| 42:DH:41:MET:SD    | 42:DH:53:GLU:N    | 2.86                     | 0.48              |
| 42:DH:70:THR:HG22  | 42:DH:74:ASN:ND2  | 2.29                     | 0.48              |
| 43:DJ:148:UNK:C    | 43:DJ:150:UNK:N   | 2.73                     | 0.48              |
| 44:DK:39:LYS:O     | 44:DK:43:ALA:HB2  | 2.13                     | 0.48              |
| 47:DO:32:TYR:CD1   | 47:DO:32:TYR:N    | 2.80                     | 0.48              |
| 35:DA:661:C:H4'    | 48:DP:18:ARG:HG2  | 1.95                     | 0.48              |
| 35:DA:2406:U:N3    | 48:DP:72:PRO:HB2  | 2.28                     | 0.48              |
| 49:DQ:108:GLY:O    | 49:DQ:109:VAL:CG2 | 2.62                     | 0.48              |
| 52:DT:57:PHE:O     | 52:DT:58:ASN:C    | 2.51                     | 0.48              |
| 52:DT:6:LEU:O      | 52:DT:7:ILE:C     | 2.51                     | 0.48              |
| 52:DT:89:VAL:C     | 52:DT:91:ARG:H    | 2.17                     | 0.48              |
| 54:DV:2:PHE:HB3    | 54:DV:41:GLY:C    | 2.34                     | 0.48              |
| 58:DZ:72:ARG:HD3   | 58:DZ:72:ARG:HA   | 1.72                     | 0.48              |
| 58:DZ:7:ALA:HA     | 58:DZ:39:VAL:HG12 | 1.95                     | 0.48              |
| 1:AA:1030(C):G:H2' | 1:AA:1030(D):A:C8 | 2.48                     | 0.48              |
| 1:AA:1134:G:N2     | 1:AA:1141:C:C2    | 2.82                     | 0.48              |
| 1:AA:961:U:OP2     | 1:AA:1223:C:H4'   | 2.13                     | 0.48              |
| 3:AC:62:ASP:O      | 3:AC:64:VAL:N     | 2.45                     | 0.48              |
| 4:AD:119:GLN:HG3   | 4:AD:123:HIS:NE2  | 2.29                     | 0.48              |
| 9:AI:20:ARG:O      | 9:AI:59:PHE:HA    | 2.14                     | 0.48              |
| 9:AI:63:ILE:HG22   | 9:AI:64:THR:N     | 2.29                     | 0.48              |
| 9:AI:5:TYR:O       | 9:AI:84:ALA:HA    | 2.14                     | 0.48              |
| 16:AP:67:THR:HG22  | 16:AP:68:ASP:N    | 2.28                     | 0.48              |
| 24:AY:21:ILE:HG13  | 35:BA:2661:G:C5'  | 2.40                     | 0.48              |
| 24:AY:346:LYS:O    | 24:AY:347:GLY:C   | 2.52                     | 0.48              |
| 24:AY:334:THR:CG2  | 24:AY:370:LYS:HG2 | 2.42                     | 0.48              |
| 24:AY:406:GLU:CB   | 24:AY:407:PRO:CD  | 2.92                     | 0.48              |
| 29:B4:22:ILE:H     | 29:B4:22:ILE:HD12 | 1.79                     | 0.48              |
| 31:B6:15:GLU:HG2   | 31:B6:16:CYS:O    | 2.13                     | 0.48              |
| 34:B9:11:CYS:O     | 34:B9:11:CYS:SG   | 2.72                     | 0.48              |
| 35:BA:1609:A:H1'   | 35:BA:1616:A:H1'  | 1.96                     | 0.48              |
| 35:BA:1629:U:H2'   | 35:BA:1630:G:C8   | 2.48                     | 0.48              |
| 35:BA:182:A:O2'    | 35:BA:183:C:H5'   | 2.13                     | 0.48              |
| 35:BA:1266:G:O2'   | 35:BA:2012:G:O6   | 2.27                     | 0.48              |
| 35:BA:2704:C:H2'   | 35:BA:2705:A:O4'  | 2.14                     | 0.48              |
| 35:BA:2886:G:H2'   | 35:BA:2887:U:C6   | 2.49                     | 0.48              |
| 35:BA:492:A:O2'    | 35:BA:493:G:H5'   | 2.14                     | 0.48              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:B7:4:THR:O     | 35:BA:687:C:H5'    | 2.14                     | 0.48              |
| 35:BA:859:G:N2    | 35:BA:917:A:OP2    | 2.27                     | 0.48              |
| 37:BC:150:ILE:O   | 37:BC:154:ILE:HG13 | 2.14                     | 0.48              |
| 37:BC:202:PRO:HB2 | 37:BC:205:ALA:HB2  | 1.95                     | 0.48              |
| 38:BD:81:ALA:HA   | 38:BD:113:VAL:CG2  | 2.44                     | 0.48              |
| 38:BD:46:GLN:OE1  | 38:BD:46:GLN:N     | 2.46                     | 0.48              |
| 35:BA:1654:A:C2   | 39:BE:113:PHE:HD1  | 2.32                     | 0.48              |
| 39:BE:36:ARG:NH2  | 39:BE:88:GLY:N     | 2.61                     | 0.48              |
| 40:BF:25:PRO:HB3  | 40:BF:119:ARG:HB2  | 1.95                     | 0.48              |
| 40:BF:81:PRO:C    | 40:BF:83:PHE:H     | 2.17                     | 0.48              |
| 41:BG:100:TRP:O   | 41:BG:101:ILE:C    | 2.52                     | 0.48              |
| 41:BG:109:VAL:CG1 | 41:BG:142:PRO:HD3  | 2.42                     | 0.48              |
| 46:BN:3:THR:CG2   | 46:BN:5:VAL:HG23   | 2.44                     | 0.48              |
| 48:BP:29:LYS:HB3  | 48:BP:34:GLY:H     | 1.79                     | 0.48              |
| 49:BQ:41:TRP:NE1  | 49:BQ:96:VAL:HG22  | 2.28                     | 0.48              |
| 51:BS:85:VAL:O    | 51:BS:106:ARG:HG2  | 2.14                     | 0.48              |
| 51:BS:44:LYS:O    | 51:BS:46:VAL:HG23  | 2.14                     | 0.48              |
| 1:CA:1489:G:C3'   | 1:CA:1490:C:H5''   | 2.42                     | 0.48              |
| 1:CA:489:C:H2'    | 1:CA:490:G:H8      | 1.79                     | 0.48              |
| 3:CC:28:GLN:O     | 3:CC:29:TYR:C      | 2.51                     | 0.48              |
| 4:CD:58:LEU:HD22  | 4:CD:59:ARG:NH1    | 2.28                     | 0.48              |
| 9:CI:59:PHE:CD1   | 9:CI:59:PHE:N      | 2.81                     | 0.48              |
| 9:CI:88:TYR:O     | 9:CI:89:ASN:CB     | 2.53                     | 0.48              |
| 12:CL:115:LYS:O   | 12:CL:117:ARG:HG3  | 2.14                     | 0.48              |
| 17:CQ:94:ASN:O    | 17:CQ:95:TYR:C     | 2.52                     | 0.48              |
| 24:CY:282:SER:C   | 24:CY:284:LEU:H    | 2.17                     | 0.48              |
| 24:CY:97:SER:O    | 24:CY:100:VAL:HG12 | 2.12                     | 0.48              |
| 29:D4:56:VAL:CG1  | 29:D4:56:VAL:O     | 2.56                     | 0.48              |
| 35:DA:1161:C:H2'  | 35:DA:1162:G:H8    | 1.79                     | 0.48              |
| 35:DA:1169:G:N2   | 35:DA:1181:C:N3    | 2.62                     | 0.48              |
| 35:DA:2245:U:C5'  | 35:DA:2246:G:H5'   | 2.35                     | 0.48              |
| 35:DA:2260:C:H2'  | 35:DA:2261:C:C6    | 2.49                     | 0.48              |
| 35:DA:2328:A:H2'  | 35:DA:2329:G:C8    | 2.48                     | 0.48              |
| 25:D0:43:THR:N    | 35:DA:2331:G:H4'   | 2.23                     | 0.48              |
| 35:DA:2836:U:H2'  | 35:DA:2837:G:C8    | 2.49                     | 0.48              |
| 35:DA:2867:G:N7   | 52:DT:23:ARG:NH1   | 2.62                     | 0.48              |
| 35:DA:391:G:O2'   | 35:DA:392:C:H5'    | 2.14                     | 0.48              |
| 35:DA:588:U:H1'   | 40:DF:90:PHE:HB3   | 1.95                     | 0.48              |
| 35:DA:619:G:H3'   | 35:DA:620:G:H21    | 1.79                     | 0.48              |
| 35:DA:946:G:H2'   | 35:DA:947:G:H8     | 1.75                     | 0.48              |
| 36:DB:106:G:H5''  | 58:DZ:31:ARG:HB3   | 1.94                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 37:DC:164:PHE:HB2 | 37:DC:172:ILE:HD11 | 1.96                     | 0.48              |
| 38:DD:24:ILE:CD1  | 38:DD:25:THR:H     | 2.24                     | 0.48              |
| 39:DE:30:PRO:O    | 39:DE:32:PRO:HD3   | 2.14                     | 0.48              |
| 41:DG:102:PHE:C   | 41:DG:104:GLU:N    | 2.67                     | 0.48              |
| 41:DG:83:ARG:HD2  | 41:DG:83:ARG:H     | 1.79                     | 0.48              |
| 41:DG:85:GLY:C    | 41:DG:87:PRO:CD    | 2.81                     | 0.48              |
| 35:DA:2531:A:H5'' | 42:DH:157:TYR:CZ   | 2.49                     | 0.48              |
| 42:DH:40:GLU:HG3  | 42:DH:64:LEU:HD13  | 1.94                     | 0.48              |
| 44:DK:37:PHE:C    | 44:DK:39:LYS:H     | 2.17                     | 0.48              |
| 44:DK:98:ARG:HD2  | 44:DK:139:VAL:HG22 | 1.96                     | 0.48              |
| 46:DN:115:ARG:HA  | 46:DN:118:LYS:HE2  | 1.94                     | 0.48              |
| 46:DN:125:GLY:HA3 | 46:DN:126:PRO:C    | 2.33                     | 0.48              |
| 48:DP:146:VAL:CG2 | 48:DP:147:LEU:H    | 2.11                     | 0.48              |
| 51:DS:25:ARG:CG   | 51:DS:26:LEU:N     | 2.77                     | 0.48              |
| 52:DT:62:THR:CG2  | 52:DT:75:ILE:HG13  | 2.44                     | 0.48              |
| 39:DE:15:PHE:CE2  | 52:DT:80:SER:HB2   | 2.49                     | 0.48              |
| 53:DU:52:ARG:O    | 53:DU:55:ARG:HG2   | 2.13                     | 0.48              |
| 57:DY:42:VAL:O    | 57:DY:65:ALA:N     | 2.39                     | 0.48              |
| 58:DZ:41:LEU:O    | 58:DZ:43:GLU:N     | 2.47                     | 0.48              |
| 58:DZ:8:TYR:CD1   | 58:DZ:8:TYR:N      | 2.81                     | 0.48              |
| 1:AA:1325:C:C2    | 1:AA:1326:C:C5     | 3.02                     | 0.48              |
| 1:AA:1376:U:H2'   | 1:AA:1377:A:C8     | 2.49                     | 0.48              |
| 1:AA:937:A:C2     | 1:AA:1379:G:O6     | 2.66                     | 0.48              |
| 1:AA:182:U:H3'    | 1:AA:183:G:C5'     | 2.44                     | 0.48              |
| 2:AB:223:ILE:O    | 2:AB:226:ARG:N     | 2.44                     | 0.48              |
| 3:AC:82:GLU:N     | 3:AC:82:GLU:CD     | 2.68                     | 0.48              |
| 4:AD:165:MET:HE2  | 4:AD:176:LEU:CD2   | 2.44                     | 0.48              |
| 4:AD:187:ARG:HH11 | 4:AD:187:ARG:HG2   | 1.79                     | 0.48              |
| 6:AF:15:ASP:C     | 6:AF:17:SER:H      | 2.17                     | 0.48              |
| 6:AF:97:PHE:O     | 18:AR:31:LEU:HD23  | 2.14                     | 0.48              |
| 7:AG:72:ARG:HG3   | 7:AG:73:MET:HG3    | 1.95                     | 0.48              |
| 15:AO:39:LEU:CD1  | 15:AO:56:LEU:HB2   | 2.43                     | 0.48              |
| 1:AA:582:U:OP1    | 15:AO:68:ARG:NH2   | 2.47                     | 0.48              |
| 18:AR:26:LEU:HD21 | 18:AR:42:ARG:NH1   | 2.29                     | 0.48              |
| 19:AS:19:VAL:CG1  | 19:AS:44:MET:HG2   | 2.43                     | 0.48              |
| 22:AW:60:A:H2'    | 22:AW:61:U:C5'     | 2.44                     | 0.48              |
| 24:AY:122:TRP:HD1 | 24:AY:123:ARG:N    | 2.12                     | 0.48              |
| 24:AY:154:GLN:CA  | 24:AY:158:GLY:HA2  | 2.43                     | 0.48              |
| 24:AY:523:PHE:CE1 | 24:AY:550:MET:SD   | 3.07                     | 0.48              |
| 24:AY:73:PHE:CE2  | 24:AY:78:ARG:HB2   | 2.49                     | 0.48              |
| 29:B4:21:VAL:O    | 29:B4:21:VAL:HG12  | 2.14                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 33:B8:21:LYS:HD3   | 33:B8:48:PHE:CE2  | 2.49                     | 0.48              |
| 35:BA:999:U:H5''   | 35:BA:1154:G:O6   | 2.14                     | 0.48              |
| 35:BA:1367:A:C2'   | 35:BA:1368:G:H5'  | 2.42                     | 0.48              |
| 35:BA:1576:U:H2'   | 35:BA:1577:C:C6   | 2.49                     | 0.48              |
| 35:BA:1829:A:N3    | 38:BD:15:PHE:HZ   | 2.10                     | 0.48              |
| 35:BA:2723:C:H5''  | 50:BR:2:ARG:NH1   | 2.17                     | 0.48              |
| 35:BA:64:A:H2'     | 35:BA:65:C:O4'    | 2.14                     | 0.48              |
| 35:BA:84:A:H5''    | 57:BY:9:LYS:HZ3   | 1.75                     | 0.48              |
| 38:BD:94:LEU:HD23  | 38:BD:95:LEU:N    | 2.29                     | 0.48              |
| 39:BE:201:THR:C    | 39:BE:202:LYS:HD2 | 2.35                     | 0.48              |
| 39:BE:51:PHE:CD1   | 39:BE:52:LEU:HD12 | 2.48                     | 0.48              |
| 41:BG:40:ASN:ND2   | 41:BG:41:GLN:H    | 2.12                     | 0.48              |
| 41:BG:53:LEU:HD22  | 41:BG:53:LEU:H    | 1.79                     | 0.48              |
| 41:BG:67:LYS:HD3   | 41:BG:68:PRO:HD2  | 1.95                     | 0.48              |
| 41:BG:71:THR:HG23  | 41:BG:90:LEU:N    | 2.29                     | 0.48              |
| 35:BA:2531:A:H5''  | 42:BH:157:TYR:CZ  | 2.49                     | 0.48              |
| 42:BH:92:ILE:C     | 42:BH:94:TYR:H    | 2.12                     | 0.48              |
| 44:BK:18:THR:C     | 44:BK:20:ALA:H    | 2.18                     | 0.48              |
| 54:BV:5:VAL:HG23   | 54:BV:37:VAL:O    | 2.13                     | 0.48              |
| 57:BY:13:VAL:HG22  | 57:BY:73:ARG:O    | 2.14                     | 0.48              |
| 1:CA:1101:A:H4'    | 1:CA:1102:A:H4'   | 1.95                     | 0.48              |
| 1:CA:1164:G:O2'    | 1:CA:1165:C:H5'   | 2.14                     | 0.48              |
| 1:CA:1237:C:H5''   | 1:CA:1238:A:C8    | 2.49                     | 0.48              |
| 1:CA:170:U:O2'     | 1:CA:171:A:H5'    | 2.14                     | 0.48              |
| 1:CA:182:U:H3'     | 1:CA:183:G:C5'    | 2.44                     | 0.48              |
| 1:CA:265:G:H5'     | 17:CQ:64:PRO:O    | 2.14                     | 0.48              |
| 1:CA:678:U:H2'     | 1:CA:679:C:C6     | 2.48                     | 0.48              |
| 8:CH:6:ILE:N       | 8:CH:6:ILE:CD1    | 2.77                     | 0.48              |
| 13:CM:63:THR:CG2   | 13:CM:64:TRP:H    | 2.24                     | 0.48              |
| 15:CO:23:GLY:O     | 15:CO:24:SER:O    | 2.32                     | 0.48              |
| 16:CP:23:ASP:OD1   | 16:CP:24:ALA:N    | 2.47                     | 0.48              |
| 16:CP:59:TRP:O     | 16:CP:62:VAL:HG22 | 2.13                     | 0.48              |
| 18:CR:53:ARG:HH21  | 18:CR:59:SER:HA   | 1.79                     | 0.48              |
| 18:CR:32:ARG:HA    | 18:CR:69:THR:HG21 | 1.95                     | 0.48              |
| 24:CY:210:ARG:NH1  | 24:CY:210:ARG:HG2 | 2.25                     | 0.48              |
| 24:CY:573:HIS:HD2  | 24:CY:576:ASP:H   | 1.61                     | 0.48              |
| 24:CY:409:ILE:HD12 | 24:CY:654:GLY:HA2 | 1.96                     | 0.48              |
| 34:D9:3:VAL:O      | 34:D9:4:ARG:HB3   | 2.14                     | 0.48              |
| 35:DA:1441:G:O2'   | 35:DA:1442:G:H5'  | 2.14                     | 0.48              |
| 35:DA:1607:C:H5'   | 35:DA:1608:A:C8   | 2.49                     | 0.48              |
| 35:DA:1810:A:H2'   | 35:DA:1811:G:O4'  | 2.14                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:2051:A:H2'   | 35:DA:2578:G:O5'   | 2.13                     | 0.48              |
| 35:DA:2463:C:C2'   | 35:DA:2464:C:H5'   | 2.43                     | 0.48              |
| 35:DA:2602:A:H4'   | 35:DA:2603:G:C5'   | 2.43                     | 0.48              |
| 35:DA:654(P):C:H2' | 35:DA:654(Q):C:O4' | 2.13                     | 0.48              |
| 35:DA:64:A:H2'     | 35:DA:65:C:O4'     | 2.14                     | 0.48              |
| 36:DB:40:U:H5''    | 36:DB:41:U:OP2     | 2.14                     | 0.48              |
| 37:DC:111:PHE:CE1  | 37:DC:137:LEU:HD13 | 2.37                     | 0.48              |
| 38:DD:211:ARG:O    | 38:DD:215:LEU:HG   | 2.13                     | 0.48              |
| 39:DE:117:MET:CA   | 39:DE:122:PHE:H    | 2.16                     | 0.48              |
| 43:DJ:139:UNK:C    | 43:DJ:141:UNK:N    | 2.77                     | 0.48              |
| 46:DN:62:VAL:HG22  | 46:DN:66:LYS:CG    | 2.39                     | 0.48              |
| 47:DO:61:VAL:N     | 47:DO:87:ILE:HD11  | 2.29                     | 0.48              |
| 48:DP:124:LYS:HD3  | 48:DP:143:GLY:CA   | 2.44                     | 0.48              |
| 48:DP:83:VAL:HG13  | 48:DP:83:VAL:O     | 2.14                     | 0.48              |
| 50:DR:12:ARG:HH11  | 50:DR:12:ARG:CG    | 2.27                     | 0.48              |
| 52:DT:102:ILE:O    | 52:DT:106:SER:HB3  | 2.14                     | 0.48              |
| 53:DU:106:PHE:HA   | 53:DU:109:LEU:HD12 | 1.96                     | 0.48              |
| 53:DU:79:PHE:HE2   | 53:DU:83:LEU:HD11  | 1.79                     | 0.48              |
| 55:DW:24:ILE:HG21  | 55:DW:36:LEU:HD21  | 1.95                     | 0.48              |
| 1:AA:1318:A:C2'    | 1:AA:1319:A:H5'    | 2.43                     | 0.47              |
| 1:AA:402:G:O2'     | 1:AA:403:C:H5'     | 2.14                     | 0.47              |
| 1:AA:408:A:OP1     | 4:AD:113:SER:OG    | 2.29                     | 0.47              |
| 1:AA:475:G:O2'     | 1:AA:476:G:H5'     | 2.13                     | 0.47              |
| 1:AA:707:C:H4'     | 11:AK:20:TYR:CD1   | 2.49                     | 0.47              |
| 2:AB:111:ARG:NH1   | 2:AB:111:ARG:HG2   | 2.29                     | 0.47              |
| 1:AA:15:G:H4'      | 5:AE:24:ARG:NH1    | 2.29                     | 0.47              |
| 6:AF:42:GLU:C      | 6:AF:44:GLY:N      | 2.68                     | 0.47              |
| 6:AF:91:VAL:CG1    | 6:AF:92:LYS:N      | 2.76                     | 0.47              |
| 12:AL:17:LYS:HD3   | 12:AL:18:VAL:N     | 2.29                     | 0.47              |
| 20:AT:53:LEU:HB3   | 20:AT:102:GLY:HA3  | 1.96                     | 0.47              |
| 20:AT:96:GLY:O     | 20:AT:97:ALA:O     | 2.31                     | 0.47              |
| 24:AY:420:ASP:N    | 24:AY:420:ASP:OD2  | 2.45                     | 0.47              |
| 24:AY:422:GLU:O    | 24:AY:425:SER:N    | 2.47                     | 0.47              |
| 24:AY:539:ILE:CA   | 24:AY:542:VAL:HG12 | 2.44                     | 0.47              |
| 35:BA:1045:A:N3    | 35:BA:1047:G:N2    | 2.62                     | 0.47              |
| 35:BA:1472:A:H2'   | 35:BA:1473:G:C8    | 2.49                     | 0.47              |
| 35:BA:1484:G:H2'   | 35:BA:1485:G:H5''  | 1.95                     | 0.47              |
| 35:BA:1528:A:H2'   | 35:BA:1528:A:N3    | 2.29                     | 0.47              |
| 35:BA:2051:A:H4'   | 39:BE:141:ILE:HD13 | 1.96                     | 0.47              |
| 35:BA:2206:G:N3    | 35:BA:2206:G:H3'   | 2.29                     | 0.47              |
| 35:BA:2463:C:C2'   | 35:BA:2464:C:H5'   | 2.44                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:2453:A:OP1   | 35:BA:2573:C:H5    | 1.96                     | 0.47              |
| 35:BA:2584:U:O4'   | 35:BA:2584:U:O2    | 2.31                     | 0.47              |
| 35:BA:41:C:H42     | 35:BA:437:G:H1     | 1.62                     | 0.47              |
| 35:BA:797:C:P      | 40:BF:62:ARG:HG3   | 2.54                     | 0.47              |
| 35:BA:799:G:OP2    | 35:BA:800:A:H3'    | 2.13                     | 0.47              |
| 25:B0:77:ARG:NH2   | 35:BA:857:C:H5'    | 2.25                     | 0.47              |
| 36:BB:53:A:N3      | 36:BB:53:A:H2'     | 2.29                     | 0.47              |
| 36:BB:74:U:H2'     | 36:BB:75:G:H5'     | 1.96                     | 0.47              |
| 35:BA:2170:A:H5''  | 37:BC:135:ARG:HE   | 1.79                     | 0.47              |
| 37:BC:225:ILE:HD12 | 37:BC:225:ILE:O    | 2.13                     | 0.47              |
| 39:BE:16:ARG:NH1   | 39:BE:171:GLU:OE2  | 2.47                     | 0.47              |
| 39:BE:24:THR:CG2   | 39:BE:186:GLY:HA2  | 2.38                     | 0.47              |
| 41:BG:138:GLN:O    | 41:BG:144:ILE:HD13 | 2.14                     | 0.47              |
| 43:BJ:125:UNK:C    | 43:BJ:127:UNK:N    | 2.76                     | 0.47              |
| 46:BN:18:ALA:O     | 46:BN:21:LYS:HB2   | 2.14                     | 0.47              |
| 47:BO:17:ARG:O     | 47:BO:18:LYS:HG3   | 2.13                     | 0.47              |
| 48:BP:89:ALA:O     | 48:BP:121:LYS:HD2  | 2.15                     | 0.47              |
| 51:BS:89:ARG:HG3   | 51:BS:92:TYR:HB3   | 1.94                     | 0.47              |
| 57:BY:56:PRO:O     | 57:BY:57:GLN:HB2   | 2.14                     | 0.47              |
| 58:BZ:151:HIS:CB   | 58:BZ:170:THR:HA   | 2.39                     | 0.47              |
| 58:BZ:84:GLU:O     | 58:BZ:85:HIS:CB    | 2.55                     | 0.47              |
| 1:CA:103:C:H3'     | 1:CA:104:G:C8      | 2.40                     | 0.47              |
| 1:CA:108:G:N2      | 1:CA:109:A:C2      | 2.82                     | 0.47              |
| 1:CA:1152:A:OP1    | 10:CJ:68:HIS:HD2   | 1.97                     | 0.47              |
| 1:CA:1237:C:H3'    | 1:CA:1336:C:H41    | 1.79                     | 0.47              |
| 1:CA:392:G:H2'     | 1:CA:393:A:C8      | 2.48                     | 0.47              |
| 1:CA:393:A:H5'     | 1:CA:483:C:O2'     | 2.14                     | 0.47              |
| 4:CD:119:GLN:HG3   | 4:CD:123:HIS:NE2   | 2.28                     | 0.47              |
| 4:CD:194:LEU:HB3   | 4:CD:196:LEU:CD1   | 2.37                     | 0.47              |
| 1:CA:430:A:OP2     | 4:CD:8:VAL:HG22    | 2.14                     | 0.47              |
| 11:CK:29:ILE:HB    | 11:CK:44:SER:HB2   | 1.96                     | 0.47              |
| 12:CL:41:ARG:HH11  | 12:CL:41:ARG:CB    | 2.18                     | 0.47              |
| 14:CN:36:PHE:CD1   | 14:CN:36:PHE:C     | 2.88                     | 0.47              |
| 19:CS:43:GLU:HB2   | 19:CS:44:MET:SD    | 2.53                     | 0.47              |
| 22:CW:10:G:O2'     | 22:CW:11:A:H5'     | 2.14                     | 0.47              |
| 24:CY:181:LEU:HD13 | 24:CY:216:LEU:HD21 | 1.96                     | 0.47              |
| 24:CY:341:VAL:HG22 | 24:CY:350:GLU:HB2  | 1.95                     | 0.47              |
| 24:CY:609:GLU:HB2  | 24:CY:670:VAL:CG2  | 2.44                     | 0.47              |
| 31:D6:19:ARG:O     | 31:D6:20:ASN:C     | 2.52                     | 0.47              |
| 35:DA:1064:C:H4'   | 44:DK:89:HIS:CD2   | 2.47                     | 0.47              |
| 35:DA:1971:A:N3    | 38:DD:240:ALA:HA   | 2.29                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:272(D):G:H1  | 35:DA:364:C:H42    | 1.62                     | 0.47              |
| 35:DA:2884:U:H2'   | 35:DA:2885:C:H5'   | 1.96                     | 0.47              |
| 35:DA:651:G:C2'    | 35:DA:652:C:H5'    | 2.43                     | 0.47              |
| 35:DA:654(P):C:H2' | 35:DA:654(Q):C:C5' | 2.44                     | 0.47              |
| 35:DA:709:U:H2'    | 35:DA:710:G:H8     | 1.77                     | 0.47              |
| 35:DA:883:G:H2'    | 35:DA:884:C:O4'    | 2.14                     | 0.47              |
| 39:DE:12:THR:O     | 39:DE:23:VAL:N     | 2.42                     | 0.47              |
| 39:DE:132:HIS:CD2  | 39:DE:135:HIS:NE2  | 2.82                     | 0.47              |
| 41:DG:172:LEU:O    | 41:DG:176:LEU:HD12 | 2.14                     | 0.47              |
| 42:DH:152:ARG:O    | 42:DH:153:LYS:C    | 2.53                     | 0.47              |
| 48:DP:64:LYS:O     | 48:DP:64:LYS:HD3   | 2.14                     | 0.47              |
| 48:DP:70:GLN:OE1   | 48:DP:70:GLN:HA    | 2.12                     | 0.47              |
| 48:DP:7:ARG:HG3    | 48:DP:7:ARG:HH11   | 1.79                     | 0.47              |
| 48:DP:83:VAL:HG13  | 48:DP:114:ILE:HA   | 1.96                     | 0.47              |
| 51:DS:74:ALA:HB2   | 51:DS:101:LEU:CD2  | 2.44                     | 0.47              |
| 51:DS:74:ALA:HB3   | 51:DS:103:GLU:HG3  | 1.95                     | 0.47              |
| 51:DS:49:VAL:HG22  | 51:DS:80:LEU:HD12  | 1.95                     | 0.47              |
| 51:DS:97:ARG:O     | 51:DS:97:ARG:NE    | 2.47                     | 0.47              |
| 52:DT:137:LYS:HG2  | 52:DT:138:ALA:N    | 2.30                     | 0.47              |
| 57:DY:31:LEU:HD23  | 57:DY:36:ALA:H     | 1.79                     | 0.47              |
| 1:AA:1225:A:H5''   | 1:AA:1226:C:OP2    | 2.14                     | 0.47              |
| 1:AA:1292:U:H2'    | 1:AA:1293:G:H8     | 1.74                     | 0.47              |
| 1:AA:533:A:OP1     | 1:AA:533:A:H3'     | 2.15                     | 0.47              |
| 1:AA:78:G:H1       | 1:AA:91:C:N4       | 2.12                     | 0.47              |
| 1:AA:930:C:O2'     | 1:AA:931:C:H5'     | 2.14                     | 0.47              |
| 2:AB:82:ARG:HH11   | 2:AB:82:ARG:HG3    | 1.79                     | 0.47              |
| 4:AD:189:PRO:HB2   | 4:AD:194:LEU:CD2   | 2.43                     | 0.47              |
| 11:AK:125:PHE:N    | 11:AK:125:PHE:CD1  | 2.82                     | 0.47              |
| 13:AM:72:ALA:O     | 13:AM:73:GLU:C     | 2.53                     | 0.47              |
| 16:AP:13:HIS:C     | 16:AP:15:PRO:HD3   | 2.34                     | 0.47              |
| 24:AY:9:LEU:C      | 24:AY:11:ARG:N     | 2.65                     | 0.47              |
| 24:AY:125:ALA:C    | 24:AY:127:LYS:H    | 2.17                     | 0.47              |
| 24:AY:217:VAL:HG22 | 24:AY:242:LEU:HD21 | 1.95                     | 0.47              |
| 24:AY:315:LYS:HD2  | 24:AY:317:MET:HG3  | 1.95                     | 0.47              |
| 24:AY:445:GLU:HA   | 24:AY:445:GLU:OE1  | 2.13                     | 0.47              |
| 24:AY:652:MET:HE2  | 24:AY:655:TYR:HB2  | 1.96                     | 0.47              |
| 25:B0:51:VAL:HG22  | 25:B0:81:VAL:CG2   | 2.44                     | 0.47              |
| 27:B2:38:GLN:C     | 27:B2:40:SER:N     | 2.67                     | 0.47              |
| 33:B8:62:LEU:N     | 33:B8:63:PRO:HD2   | 2.29                     | 0.47              |
| 34:B9:16:VAL:HA    | 34:B9:25:VAL:HG22  | 1.95                     | 0.47              |
| 35:BA:1708:C:O2'   | 35:BA:1709:U:H5'   | 2.14                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 35:BA:1799:G:H5'    | 35:BA:1819:A:H61   | 1.79                     | 0.47              |
| 35:BA:2400:G:N2     | 35:BA:2417:C:C2    | 2.82                     | 0.47              |
| 35:BA:25:U:H2'      | 35:BA:26:G:O4'     | 2.13                     | 0.47              |
| 30:B5:22:HIS:CE1    | 35:BA:2624:G:H1'   | 2.49                     | 0.47              |
| 35:BA:2704:C:O2'    | 35:BA:2705:A:H5'   | 2.14                     | 0.47              |
| 35:BA:2860:A:H2'    | 35:BA:2861:G:H5'   | 1.95                     | 0.47              |
| 35:BA:614:U:H2'     | 35:BA:614(A):U:O4' | 2.14                     | 0.47              |
| 35:BA:925:C:C3'     | 35:BA:926:A:H5''   | 2.43                     | 0.47              |
| 27:B2:47:ASN:CB     | 35:BA:95:G:H1'     | 2.44                     | 0.47              |
| 39:BE:145:LYS:O     | 39:BE:148:GLY:N    | 2.47                     | 0.47              |
| 35:BA:2784:C:H1'    | 39:BE:37:ARG:HH12  | 1.78                     | 0.47              |
| 41:BG:114:ILE:O     | 41:BG:116:ASP:N    | 2.39                     | 0.47              |
| 46:BN:9:VAL:HG12    | 46:BN:10:GLU:H     | 1.77                     | 0.47              |
| 35:BA:385:C:O2      | 48:BP:71:VAL:HG21  | 2.14                     | 0.47              |
| 49:BQ:21:THR:CG2    | 49:BQ:101:ARG:HB2  | 2.44                     | 0.47              |
| 49:BQ:50:ALA:O      | 49:BQ:51:ARG:C     | 2.52                     | 0.47              |
| 51:BS:59:LYS:HG2    | 51:BS:60:GLY:H     | 1.79                     | 0.47              |
| 54:BV:4:ILE:O       | 54:BV:4:ILE:HG22   | 2.13                     | 0.47              |
| 55:BW:20:VAL:O      | 55:BW:23:LEU:N     | 2.46                     | 0.47              |
| 57:BY:61:ILE:CG1    | 57:BY:62:GLU:N     | 2.77                     | 0.47              |
| 58:BZ:81:ARG:O      | 58:BZ:81:ARG:HG3   | 2.14                     | 0.47              |
| 1:CA:1444:C:C2      | 1:CA:1445:C:C5     | 3.01                     | 0.47              |
| 3:CC:90:GLU:C       | 3:CC:93:LYS:HB3    | 2.34                     | 0.47              |
| 4:CD:36:ARG:HH11    | 4:CD:36:ARG:CG     | 2.27                     | 0.47              |
| 9:CI:20:ARG:O       | 9:CI:59:PHE:HA     | 2.13                     | 0.47              |
| 10:CJ:33:GLN:H      | 10:CJ:75:ILE:HD11  | 1.79                     | 0.47              |
| 10:CJ:54:PHE:O      | 10:CJ:55:LYS:C     | 2.53                     | 0.47              |
| 16:CP:32:TYR:O      | 16:CP:32:TYR:CD2   | 2.62                     | 0.47              |
| 19:CS:10:PHE:HZ     | 19:CS:70:LYS:HZ3   | 1.62                     | 0.47              |
| 24:CY:20:HIS:N      | 24:CY:121:VAL:HG11 | 2.29                     | 0.47              |
| 24:CY:288:PRO:HB3   | 24:CY:301:ILE:O    | 2.14                     | 0.47              |
| 24:CY:460:GLU:O     | 24:CY:463:VAL:HB   | 2.14                     | 0.47              |
| 24:CY:74:TRP:CE2    | 24:CY:273:LEU:HB3  | 2.49                     | 0.47              |
| 35:DA:1050:A:H2'    | 35:DA:1051:G:O4'   | 2.14                     | 0.47              |
| 35:DA:1285:G:C2'    | 35:DA:1286:A:H5'   | 2.36                     | 0.47              |
| 35:DA:1445(A):C:H5' | 35:DA:1446:C:OP2   | 2.14                     | 0.47              |
| 35:DA:2223:G:H2'    | 35:DA:2224:G:H5'   | 1.96                     | 0.47              |
| 35:DA:2313:C:O2'    | 35:DA:2314:C:H5'   | 2.15                     | 0.47              |
| 35:DA:2395:C:C2     | 35:DA:2396:G:C8    | 3.02                     | 0.47              |
| 35:DA:2593:U:C2     | 35:DA:2594:C:C5    | 3.02                     | 0.47              |
| 35:DA:2735:G:H2'    | 35:DA:2736:G:C8    | 2.44                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 32:D7:5:TRP:CH2    | 35:DA:686:G:N7    | 2.82                     | 0.47              |
| 35:DA:962:G:C2'    | 35:DA:963:U:H5'   | 2.43                     | 0.47              |
| 37:DC:185:LYS:CA   | 37:DC:185:LYS:HE3 | 2.44                     | 0.47              |
| 38:DD:46:GLN:OE1   | 38:DD:46:GLN:N    | 2.48                     | 0.47              |
| 38:DD:77:ALA:HB2   | 38:DD:97:TYR:CG   | 2.49                     | 0.47              |
| 46:DN:65:LYS:CB    | 46:DN:69:GLN:HG3  | 2.41                     | 0.47              |
| 47:DO:19:ILE:HD12  | 47:DO:41:ALA:CB   | 2.45                     | 0.47              |
| 48:DP:100:LEU:HD22 | 48:DP:100:LEU:N   | 2.29                     | 0.47              |
| 49:DQ:26:TYR:CE1   | 49:DQ:140:ALA:HB3 | 2.49                     | 0.47              |
| 49:DQ:55:VAL:HG12  | 49:DQ:56:ARG:H    | 1.79                     | 0.47              |
| 53:DU:8:VAL:CG2    | 53:DU:12:ARG:HE   | 2.27                     | 0.47              |
| 53:DU:90:VAL:HG13  | 54:DV:39:LEU:HG   | 1.95                     | 0.47              |
| 54:DV:38:LEU:HD12  | 54:DV:56:SER:HA   | 1.96                     | 0.47              |
| 58:DZ:89:PHE:CE1   | 58:DZ:96:VAL:HG21 | 2.48                     | 0.47              |
| 1:AA:1268:A:H2'    | 1:AA:1269:A:C8    | 2.48                     | 0.47              |
| 1:AA:1368:G:OP2    | 9:AI:112:LYS:HD3  | 2.14                     | 0.47              |
| 1:AA:1442:G:C5     | 1:AA:1442(B):A:C2 | 3.02                     | 0.47              |
| 1:AA:1484:C:H2'    | 1:AA:1485:U:O4'   | 2.15                     | 0.47              |
| 1:AA:17:U:H2'      | 1:AA:18:C:C6      | 2.49                     | 0.47              |
| 1:AA:936:C:H2'     | 1:AA:937:A:O4'    | 2.14                     | 0.47              |
| 3:AC:173:VAL:HG12  | 3:AC:175:LEU:CD1  | 2.44                     | 0.47              |
| 4:AD:158:ILE:CG2   | 4:AD:162:LEU:HD12 | 2.43                     | 0.47              |
| 4:AD:74:GLN:HA     | 4:AD:77:ASN:HD22  | 1.78                     | 0.47              |
| 5:AE:122:GLU:O     | 5:AE:123:LEU:HD23 | 2.14                     | 0.47              |
| 9:AI:5:TYR:CG      | 9:AI:6:GLY:N      | 2.82                     | 0.47              |
| 11:AK:34:ASP:CB    | 11:AK:35:PRO:CD   | 2.93                     | 0.47              |
| 11:AK:15:ALA:HA    | 11:AK:76:GLY:O    | 2.14                     | 0.47              |
| 1:AA:502:G:OP1     | 12:AL:118:SER:HB3 | 2.14                     | 0.47              |
| 19:AS:15:LEU:O     | 19:AS:19:VAL:HB   | 2.14                     | 0.47              |
| 19:AS:58:VAL:O     | 19:AS:60:VAL:N    | 2.47                     | 0.47              |
| 22:AW:29:C:O2'     | 22:AW:30:G:H5'    | 2.14                     | 0.47              |
| 24:AY:139:MET:HE1  | 24:AY:146:LEU:HB2 | 1.96                     | 0.47              |
| 24:AY:259:PHE:N    | 24:AY:259:PHE:CD1 | 2.81                     | 0.47              |
| 24:AY:385:THR:OG1  | 24:AY:386:GLY:N   | 2.47                     | 0.47              |
| 24:AY:528:ALA:O    | 24:AY:568:TYR:HA  | 2.14                     | 0.47              |
| 24:AY:637:ARG:O    | 24:AY:638:GLY:C   | 2.52                     | 0.47              |
| 24:AY:610:VAL:HG23 | 24:AY:643:ILE:HB  | 1.95                     | 0.47              |
| 26:B1:18:ILE:HD11  | 26:B1:37:ILE:HG12 | 1.96                     | 0.47              |
| 26:B1:51:VAL:O     | 26:B1:58:ILE:HG22 | 2.14                     | 0.47              |
| 29:B4:39:CYS:O     | 29:B4:42:PHE:CE2  | 2.67                     | 0.47              |
| 29:B4:43:TYR:HD2   | 29:B4:44:THR:HG23 | 1.79                     | 0.47              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:B5:16:ARG:HD2   | 30:B5:20:ARG:HH12  | 1.79                     | 0.47              |
| 30:B5:35:GLU:O     | 30:B5:36:CYS:CB    | 2.62                     | 0.47              |
| 31:B6:6:ARG:O      | 31:B6:7:ILE:CB     | 2.62                     | 0.47              |
| 31:B6:10:LEU:HB3   | 33:B8:34:TRP:CD1   | 2.49                     | 0.47              |
| 35:BA:1181:C:O2'   | 35:BA:1182:A:H5'   | 2.14                     | 0.47              |
| 35:BA:1658:C:O5'   | 35:BA:1658:C:H6    | 1.97                     | 0.47              |
| 35:BA:1719:G:H2'   | 35:BA:1720:U:H5'   | 1.96                     | 0.47              |
| 35:BA:2759:G:O2'   | 35:BA:2760:C:H5'   | 2.14                     | 0.47              |
| 35:BA:883:G:H2'    | 35:BA:884:C:O4'    | 2.14                     | 0.47              |
| 36:BB:86:G:C6      | 36:BB:92:C:N3      | 2.82                     | 0.47              |
| 37:BC:164:PHE:HB2  | 37:BC:172:ILE:HD11 | 1.96                     | 0.47              |
| 37:BC:85:LYS:O     | 37:BC:89:GLU:HG3   | 2.14                     | 0.47              |
| 38:BD:229:VAL:HG23 | 38:BD:230:ASP:N    | 2.28                     | 0.47              |
| 38:BD:26:LYS:O     | 38:BD:27:THR:HB    | 2.13                     | 0.47              |
| 39:BE:103:ASP:OD2  | 39:BE:201:THR:HA   | 2.14                     | 0.47              |
| 39:BE:110:GLY:O    | 50:BR:2:ARG:HD3    | 2.14                     | 0.47              |
| 39:BE:188:VAL:HG23 | 39:BE:189:PRO:HD2  | 1.97                     | 0.47              |
| 41:BG:41:GLN:HB3   | 41:BG:43:LEU:CD2   | 2.44                     | 0.47              |
| 46:BN:125:GLY:CA   | 46:BN:126:PRO:O    | 2.62                     | 0.47              |
| 47:BO:17:ARG:HH21  | 47:BO:47:ILE:HD11  | 1.79                     | 0.47              |
| 48:BP:70:GLN:HA    | 48:BP:70:GLN:OE1   | 2.12                     | 0.47              |
| 49:BQ:26:TYR:CE1   | 49:BQ:140:ALA:HB3  | 2.49                     | 0.47              |
| 49:BQ:32:TYR:N     | 49:BQ:32:TYR:CD1   | 2.83                     | 0.47              |
| 50:BR:96:ARG:O     | 50:BR:114:VAL:HA   | 2.14                     | 0.47              |
| 50:BR:83:ILE:O     | 50:BR:87:TYR:CE2   | 2.67                     | 0.47              |
| 51:BS:70:GLY:O     | 51:BS:72:ALA:N     | 2.47                     | 0.47              |
| 52:BT:118:ARG:HA   | 52:BT:121:ILE:HD12 | 1.96                     | 0.47              |
| 39:BE:15:PHE:CE2   | 52:BT:80:SER:HB2   | 2.49                     | 0.47              |
| 58:BZ:108:PRO:HB3  | 58:BZ:141:VAL:HG12 | 1.95                     | 0.47              |
| 1:CA:1318:A:C2'    | 1:CA:1319:A:H5'    | 2.44                     | 0.47              |
| 1:CA:1354:C:H2'    | 1:CA:1355:G:H8     | 1.79                     | 0.47              |
| 1:CA:360:A:O2'     | 1:CA:361:G:H5'     | 2.14                     | 0.47              |
| 1:CA:392:G:H2'     | 1:CA:393:A:H8      | 1.79                     | 0.47              |
| 1:CA:763:G:H2'     | 1:CA:764:C:H6      | 1.80                     | 0.47              |
| 5:CE:119:LEU:N     | 5:CE:119:LEU:HD23  | 2.29                     | 0.47              |
| 9:CI:79:LEU:O      | 9:CI:80:GLY:C      | 2.51                     | 0.47              |
| 10:CJ:32:ALA:N     | 10:CJ:78:ASN:HD21  | 2.11                     | 0.47              |
| 11:CK:125:PHE:CD1  | 11:CK:125:PHE:N    | 2.83                     | 0.47              |
| 12:CL:117:ARG:O    | 12:CL:119:LYS:O    | 2.32                     | 0.47              |
| 14:CN:48:ALA:HB2   | 14:CN:53:LEU:HD12  | 1.95                     | 0.47              |
| 24:CY:427:ALA:HB1  | 24:CY:466:LEU:CD1  | 2.44                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:CY:532:GLY:C    | 24:CY:534:ILE:N    | 2.67                     | 0.47              |
| 24:CY:5:VAL:CG1    | 24:CY:6:GLU:H      | 2.22                     | 0.47              |
| 24:CY:91:THR:O     | 24:CY:92:ILE:C     | 2.52                     | 0.47              |
| 26:D1:76:ARG:HH22  | 26:D1:95:LEU:CG    | 2.27                     | 0.47              |
| 27:D2:27:GLU:O     | 27:D2:30:ARG:N     | 2.47                     | 0.47              |
| 30:D5:2:ALA:O      | 30:D5:3:LYS:HB3    | 2.13                     | 0.47              |
| 31:D6:47:THR:CG2   | 31:D6:49:HIS:CE1   | 2.97                     | 0.47              |
| 32:D7:16:HIS:ND1   | 35:DA:684:G:OP1    | 2.47                     | 0.47              |
| 33:D8:62:LEU:N     | 33:D8:63:PRO:HD2   | 2.29                     | 0.47              |
| 35:DA:999:U:OP2    | 35:DA:1153:C:OP2   | 2.32                     | 0.47              |
| 35:DA:2134:A:H2'   | 35:DA:2134:A:N3    | 2.29                     | 0.47              |
| 35:DA:2150:U:H2'   | 35:DA:2151:G:H8    | 1.79                     | 0.47              |
| 35:DA:2573:C:OP1   | 35:DA:2575:C:OP2   | 2.33                     | 0.47              |
| 35:DA:2888:C:H2'   | 35:DA:2889:C:C6    | 2.48                     | 0.47              |
| 37:DC:79:ALA:HB1   | 37:DC:83:LYS:HB2   | 1.95                     | 0.47              |
| 40:DF:156:LEU:HD21 | 40:DF:163:VAL:HG12 | 1.95                     | 0.47              |
| 42:DH:72:ILE:O     | 42:DH:75:ALA:N     | 2.47                     | 0.47              |
| 48:DP:17:LYS:O     | 48:DP:17:LYS:HG2   | 2.14                     | 0.47              |
| 35:DA:2394:C:P     | 48:DP:63:PRO:HD2   | 2.54                     | 0.47              |
| 49:DQ:50:ALA:O     | 49:DQ:51:ARG:C     | 2.52                     | 0.47              |
| 51:DS:12:PHE:CD1   | 51:DS:12:PHE:C     | 2.87                     | 0.47              |
| 53:DU:64:ARG:O     | 53:DU:65:ILE:C     | 2.53                     | 0.47              |
| 53:DU:70:ARG:NH2   | 53:DU:75:ASN:HB2   | 2.29                     | 0.47              |
| 53:DU:95:LEU:O     | 53:DU:98:LEU:HG    | 2.14                     | 0.47              |
| 57:DY:28:LYS:HE3   | 57:DY:30:VAL:HG22  | 1.95                     | 0.47              |
| 57:DY:95:LYS:HD3   | 57:DY:100:ALA:CB   | 2.44                     | 0.47              |
| 58:DZ:166:SER:CB   | 58:DZ:168:GLU:N    | 2.76                     | 0.47              |
| 58:DZ:9:TYR:HB3    | 58:DZ:35:ARG:HH22  | 1.78                     | 0.47              |
| 1:AA:1293:G:O2'    | 1:AA:1294:G:H5'    | 2.14                     | 0.47              |
| 1:AA:509:A:N3      | 1:AA:509:A:H2'     | 2.30                     | 0.47              |
| 1:AA:736:C:H2'     | 1:AA:737:A:H8      | 1.77                     | 0.47              |
| 2:AB:109:SER:O     | 2:AB:112:VAL:HB    | 2.14                     | 0.47              |
| 2:AB:22:LYS:HE2    | 2:AB:22:LYS:CA     | 2.36                     | 0.47              |
| 2:AB:8:LYS:HB2     | 2:AB:9:GLU:OE2     | 2.14                     | 0.47              |
| 4:AD:13:ARG:HD2    | 4:AD:38:TYR:O      | 2.15                     | 0.47              |
| 6:AF:99:ALA:O      | 6:AF:100:ASN:HB2   | 2.14                     | 0.47              |
| 7:AG:31:MET:SD     | 7:AG:36:LYS:HB2    | 2.53                     | 0.47              |
| 10:AJ:22:LYS:HZ2   | 10:AJ:88:LEU:HD23  | 1.80                     | 0.47              |
| 11:AK:24:SER:O     | 11:AK:88:GLY:HA2   | 2.14                     | 0.47              |
| 1:AA:881:G:P       | 12:AL:12:ARG:HH22  | 2.37                     | 0.47              |
| 17:AQ:45:HIS:CG    | 17:AQ:65:ILE:HD13  | 2.49                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 17:AQ:45:HIS:HB2  | 17:AQ:65:ILE:HD13  | 1.97                     | 0.47              |
| 17:AQ:50:LYS:O    | 17:AQ:50:LYS:HG3   | 2.15                     | 0.47              |
| 19:AS:48:THR:HG22 | 19:AS:61:TYR:HD1   | 1.80                     | 0.47              |
| 22:AW:75:C:H5'    | 22:AW:75:C:C6      | 2.48                     | 0.47              |
| 24:AY:176:GLY:HA2 | 24:AY:187:THR:HA   | 1.95                     | 0.47              |
| 24:AY:221:ALA:C   | 24:AY:223:PHE:H    | 2.18                     | 0.47              |
| 24:AY:590:ILE:C   | 24:AY:592:GLU:H    | 2.18                     | 0.47              |
| 24:AY:555:LEU:CD1 | 24:AY:599:PRO:HB2  | 2.43                     | 0.47              |
| 31:B6:27:LYS:HZ2  | 31:B6:30:THR:CB    | 2.27                     | 0.47              |
| 32:B7:41:ARG:NH2  | 35:BA:460:A:OP1    | 2.48                     | 0.47              |
| 33:B8:39:LYS:HG3  | 33:B8:43:GLN:NE2   | 2.30                     | 0.47              |
| 35:BA:1175:U:H4'  | 35:BA:1176:G:H5'   | 1.96                     | 0.47              |
| 35:BA:1336:A:O2'  | 35:BA:1337:G:H5'   | 2.14                     | 0.47              |
| 35:BA:1577:C:H2'  | 35:BA:1578:U:O4'   | 2.15                     | 0.47              |
| 35:BA:1661:G:O2'  | 35:BA:1662:C:H5'   | 2.14                     | 0.47              |
| 35:BA:2116:G:N7   | 35:BA:2117:A:C5    | 2.82                     | 0.47              |
| 35:BA:2794:C:H42  | 35:BA:2801(A):A:N6 | 2.11                     | 0.47              |
| 35:BA:307:G:H21   | 35:BA:330:A:N6     | 2.13                     | 0.47              |
| 35:BA:583:G:H2'   | 35:BA:584:C:H6     | 1.78                     | 0.47              |
| 35:BA:588:U:H2'   | 35:BA:589:C:H6     | 1.78                     | 0.47              |
| 35:BA:733:G:C6    | 35:BA:761:A:N7     | 2.83                     | 0.47              |
| 35:BA:809:G:O2'   | 35:BA:810:U:H5'    | 2.14                     | 0.47              |
| 37:BC:14:LYS:O    | 37:BC:15:VAL:HG13  | 2.14                     | 0.47              |
| 37:BC:65:LEU:HD11 | 37:BC:162:ILE:HD13 | 1.96                     | 0.47              |
| 35:BA:1675:C:O2   | 39:BE:129:HIS:HA   | 2.14                     | 0.47              |
| 40:BF:204:ASN:C   | 40:BF:206:ILE:H    | 2.17                     | 0.47              |
| 41:BG:117:PHE:HE1 | 41:BG:120:LEU:N    | 2.12                     | 0.47              |
| 41:BG:125:PHE:CE1 | 41:BG:131:TYR:HD1  | 2.32                     | 0.47              |
| 42:BH:146:ALA:O   | 42:BH:149:ARG:N    | 2.47                     | 0.47              |
| 42:BH:89:ILE:O    | 42:BH:89:ILE:CG1   | 2.62                     | 0.47              |
| 44:BK:6:ALA:CB    | 44:BK:30:HIS:HE1   | 2.28                     | 0.47              |
| 44:BK:69:THR:C    | 44:BK:70:LYS:HE3   | 2.35                     | 0.47              |
| 49:BQ:35:VAL:O    | 49:BQ:129:THR:HG22 | 2.15                     | 0.47              |
| 50:BR:87:TYR:C    | 50:BR:89:ASP:N     | 2.66                     | 0.47              |
| 51:BS:36:TYR:HD1  | 51:BS:36:TYR:N     | 2.12                     | 0.47              |
| 52:BT:99:LEU:HB2  | 52:BT:101:PHE:HE1  | 1.80                     | 0.47              |
| 52:BT:128:GLU:OE2 | 52:BT:129:ARG:N    | 2.48                     | 0.47              |
| 54:BV:2:PHE:O     | 54:BV:3:ALA:CB     | 2.63                     | 0.47              |
| 54:BV:40:LEU:CA   | 54:BV:45:THR:HB    | 2.40                     | 0.47              |
| 55:BW:88:ARG:CB   | 55:BW:92:ARG:HB3   | 2.44                     | 0.47              |
| 57:BY:85:VAL:HG13 | 57:BY:93:GLY:O     | 2.13                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1134:G:N2     | 1:CA:1141:C:C2     | 2.83                     | 0.47              |
| 1:CA:164:U:H2'     | 1:CA:165:C:H6      | 1.79                     | 0.47              |
| 1:CA:265:G:O2'     | 1:CA:266:G:H5'     | 2.14                     | 0.47              |
| 1:CA:417:C:H2'     | 1:CA:418:C:H6      | 1.79                     | 0.47              |
| 1:CA:603:U:H2'     | 1:CA:604:G:H8      | 1.78                     | 0.47              |
| 1:CA:608:A:O2'     | 1:CA:609:A:H5'     | 2.15                     | 0.47              |
| 2:CB:179:LYS:O     | 2:CB:179:LYS:HG2   | 2.14                     | 0.47              |
| 3:CC:130:VAL:O     | 3:CC:134:ILE:HG13  | 2.14                     | 0.47              |
| 1:CA:542:G:P       | 4:CD:10:ARG:HH21   | 2.38                     | 0.47              |
| 4:CD:13:ARG:HD2    | 4:CD:38:TYR:O      | 2.14                     | 0.47              |
| 4:CD:25:ARG:O      | 4:CD:28:SER:N      | 2.48                     | 0.47              |
| 6:CF:29:ALA:O      | 6:CF:31:GLU:N      | 2.48                     | 0.47              |
| 6:CF:43:LEU:H      | 6:CF:43:LEU:CD1    | 2.20                     | 0.47              |
| 8:CH:44:PHE:HE2    | 8:CH:109:ILE:CG2   | 2.28                     | 0.47              |
| 8:CH:19:VAL:CG2    | 8:CH:21:LYS:HE2    | 2.44                     | 0.47              |
| 9:CI:9:ARG:HG2     | 9:CI:14:VAL:HA     | 1.96                     | 0.47              |
| 10:CJ:69:ASN:O     | 10:CJ:70:ARG:HG3   | 2.15                     | 0.47              |
| 11:CK:23:ALA:O     | 11:CK:86:GLY:HA3   | 2.14                     | 0.47              |
| 15:CO:9:GLN:O      | 15:CO:10:LYS:C     | 2.52                     | 0.47              |
| 16:CP:15:PRO:O     | 16:CP:16:HIS:ND1   | 2.48                     | 0.47              |
| 18:CR:59:SER:H     | 18:CR:62:GLU:CB    | 2.25                     | 0.47              |
| 18:CR:88:LYS:HD3   | 18:CR:88:LYS:C     | 2.34                     | 0.47              |
| 22:CV:29:G:O2'     | 22:CV:30:G:H5'     | 2.15                     | 0.47              |
| 24:CY:121:VAL:HG23 | 24:CY:122:TRP:N    | 2.29                     | 0.47              |
| 24:CY:168:ILE:HD11 | 24:CY:178:ILE:HD11 | 1.95                     | 0.47              |
| 24:CY:74:TRP:NE1   | 24:CY:273:LEU:HB3  | 2.29                     | 0.47              |
| 24:CY:286:ILE:HD12 | 24:CY:286:ILE:N    | 2.29                     | 0.47              |
| 24:CY:92:ILE:HG12  | 24:CY:405:PRO:HG2  | 1.91                     | 0.47              |
| 24:CY:491:VAL:CG2  | 24:CY:597:GLY:HA2  | 2.44                     | 0.47              |
| 24:CY:510:VAL:HG11 | 24:CY:567:LEU:HD13 | 1.95                     | 0.47              |
| 24:CY:652:MET:HA   | 24:CY:652:MET:HE2  | 1.96                     | 0.47              |
| 24:CY:26:THR:HB    | 62:CY:703:GDP:O2A  | 2.14                     | 0.47              |
| 25:D0:23:VAL:HG13  | 25:D0:38:VAL:HG22  | 1.97                     | 0.47              |
| 29:D4:39:CYS:O     | 29:D4:42:PHE:CE2   | 2.67                     | 0.47              |
| 30:D5:16:ARG:NH1   | 30:D5:17:ASP:OD1   | 2.48                     | 0.47              |
| 30:D5:44:THR:CG2   | 30:D5:45:VAL:H     | 2.23                     | 0.47              |
| 31:D6:28:ARG:O     | 31:D6:32:ASN:HB2   | 2.14                     | 0.47              |
| 31:D6:6:ARG:C      | 31:D6:8:LYS:H      | 2.15                     | 0.47              |
| 33:D8:29:LYS:HD2   | 33:D8:44:LYS:CB    | 2.44                     | 0.47              |
| 35:DA:1288:U:H4'   | 35:DA:1289:C:OP2   | 2.14                     | 0.47              |
| 35:DA:1582:C:H2'   | 35:DA:1583:A:C8    | 2.43                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:1629:U:H2'   | 35:DA:1630:G:C8    | 2.50                     | 0.47              |
| 35:DA:177:G:H3'    | 35:DA:178:G:H8     | 1.79                     | 0.47              |
| 35:DA:1851:U:H2'   | 35:DA:1852:C:O4'   | 2.14                     | 0.47              |
| 35:DA:1899:G:N2    | 35:DA:1902:C:C4    | 2.80                     | 0.47              |
| 35:DA:393:C:O2'    | 35:DA:394:A:H5'    | 2.13                     | 0.47              |
| 35:DA:544:G:H21    | 35:DA:547:A:H2'    | 1.79                     | 0.47              |
| 35:DA:750:A:C2     | 35:DA:753:C:C6     | 3.02                     | 0.47              |
| 35:DA:799:G:C3'    | 35:DA:800:A:H5''   | 2.43                     | 0.47              |
| 35:DA:848:G:C4     | 35:DA:933:A:H8     | 2.32                     | 0.47              |
| 37:DC:182:PRO:HD2  | 37:DC:185:LYS:HG2  | 1.96                     | 0.47              |
| 38:DD:28:GLU:HB2   | 38:DD:29:PRO:HD3   | 1.96                     | 0.47              |
| 39:DE:93:VAL:C     | 39:DE:95:ILE:N     | 2.67                     | 0.47              |
| 41:DG:39:ILE:HD11  | 41:DG:92:VAL:HG23  | 1.95                     | 0.47              |
| 44:DK:5:VAL:HG12   | 44:DK:59:ILE:HG23  | 1.96                     | 0.47              |
| 49:DQ:43:THR:HB    | 49:DQ:45:GLN:HE21  | 1.80                     | 0.47              |
| 35:DA:2334:G:C2    | 51:DS:15:ARG:NH1   | 2.83                     | 0.47              |
| 51:DS:70:GLY:C     | 51:DS:72:ALA:N     | 2.68                     | 0.47              |
| 51:DS:85:VAL:HG23  | 51:DS:106:ARG:CG   | 2.42                     | 0.47              |
| 54:DV:40:LEU:N     | 54:DV:40:LEU:HD22  | 2.29                     | 0.47              |
| 54:DV:46:VAL:O     | 54:DV:47:VAL:HG13  | 2.15                     | 0.47              |
| 1:AA:624:C:H2'     | 1:AA:625:G:C8      | 2.47                     | 0.47              |
| 1:AA:710:G:O2'     | 1:AA:711:G:H5'     | 2.14                     | 0.47              |
| 1:AA:830:G:O2'     | 1:AA:831:U:H5'     | 2.14                     | 0.47              |
| 8:AH:19:VAL:HG21   | 8:AH:21:LYS:HE2    | 1.96                     | 0.47              |
| 9:AI:33:PHE:C      | 9:AI:35:GLU:H      | 2.18                     | 0.47              |
| 9:AI:4:TYR:CE1     | 9:AI:88:TYR:CD2    | 3.03                     | 0.47              |
| 12:AL:6:THR:HG23   | 12:AL:9:GLN:NE2    | 2.21                     | 0.47              |
| 15:AO:25:THR:O     | 15:AO:26:GLU:C     | 2.53                     | 0.47              |
| 16:AP:67:THR:HB    | 16:AP:70:ALA:HB2   | 1.97                     | 0.47              |
| 1:AA:1352:C:OP1    | 21:AU:3:LYS:HE2    | 2.15                     | 0.47              |
| 24:AY:9:LEU:HD23   | 24:AY:10:LYS:N     | 2.28                     | 0.47              |
| 24:AY:198:GLU:O    | 24:AY:198:GLU:HG3  | 2.13                     | 0.47              |
| 24:AY:210:ARG:HH11 | 24:AY:210:ARG:HG2  | 1.79                     | 0.47              |
| 24:AY:282:SER:O    | 24:AY:286:ILE:HD13 | 2.14                     | 0.47              |
| 31:B6:9:LEU:C      | 31:B6:9:LEU:HD22   | 2.34                     | 0.47              |
| 35:BA:1050:A:H2'   | 35:BA:1051:G:O4'   | 2.14                     | 0.47              |
| 35:BA:1150:C:O2'   | 35:BA:1151:G:H5'   | 2.15                     | 0.47              |
| 35:BA:1166:C:H2'   | 35:BA:1167:U:C6    | 2.49                     | 0.47              |
| 35:BA:1310:G:H2'   | 35:BA:1311:G:H5'   | 1.96                     | 0.47              |
| 35:BA:1582:C:O2'   | 35:BA:1586:A:C8    | 2.66                     | 0.47              |
| 35:BA:2552:U:H6    | 35:BA:2552:U:O5'   | 1.98                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:BA:2656:U:N3    | 35:BA:2665:A:H2   | 2.12                     | 0.47              |
| 35:BA:2695:C:H2'   | 35:BA:2696:U:C6   | 2.49                     | 0.47              |
| 35:BA:537:C:H2'    | 35:BA:538:G:C8    | 2.50                     | 0.47              |
| 35:BA:582:G:C6     | 35:BA:1259:G:N1   | 2.83                     | 0.47              |
| 35:BA:979:G:N2     | 35:BA:985:C:N4    | 2.62                     | 0.47              |
| 38:BD:24:ILE:CD1   | 38:BD:25:THR:H    | 2.22                     | 0.47              |
| 38:BD:34:VAL:O     | 38:BD:36:PRO:HG2  | 2.15                     | 0.47              |
| 40:BF:199:TRP:O    | 40:BF:202:PHE:HB3 | 2.14                     | 0.47              |
| 48:BP:83:VAL:HG13  | 48:BP:114:ILE:HA  | 1.96                     | 0.47              |
| 49:BQ:110:THR:CG2  | 49:BQ:113:GLN:HG3 | 2.44                     | 0.47              |
| 53:BU:47:TYR:O     | 53:BU:51:LYS:HG2  | 2.14                     | 0.47              |
| 54:BV:39:LEU:HA    | 54:BV:47:VAL:CG1  | 2.44                     | 0.47              |
| 54:BV:88:ARG:O     | 54:BV:90:PRO:HD3  | 2.15                     | 0.47              |
| 57:BY:49:VAL:O     | 57:BY:51:VAL:HG23 | 2.15                     | 0.47              |
| 35:BA:328:U:H4'    | 57:BY:68:HIS:NE2  | 2.29                     | 0.47              |
| 1:CA:1299:A:C2     | 1:CA:1301:U:N3    | 2.82                     | 0.47              |
| 1:CA:538:G:O2'     | 1:CA:539:A:H5'    | 2.14                     | 0.47              |
| 1:CA:59:A:H5''     | 1:CA:60:A:H5'     | 1.96                     | 0.47              |
| 1:CA:930:C:C2'     | 1:CA:931:C:H5'    | 2.45                     | 0.47              |
| 3:CC:134:ILE:HD11  | 3:CC:153:VAL:CG2  | 2.43                     | 0.47              |
| 5:CE:78:HIS:HE1    | 5:CE:80:ILE:HG23  | 1.79                     | 0.47              |
| 8:CH:85:ARG:HG3    | 8:CH:85:ARG:HH11  | 1.80                     | 0.47              |
| 17:CQ:67:LYS:CA    | 17:CQ:70:ARG:HH12 | 2.24                     | 0.47              |
| 17:CQ:59:ILE:CG2   | 17:CQ:71:PHE:HB3  | 2.39                     | 0.47              |
| 20:CT:33:ILE:HG21  | 20:CT:63:ILE:HG12 | 1.95                     | 0.47              |
| 24:CY:518:PRO:O    | 24:CY:519:ARG:C   | 2.52                     | 0.47              |
| 29:D4:7:PRO:HG2    | 41:DG:61:ALA:HB1  | 1.96                     | 0.47              |
| 30:D5:3:LYS:CE     | 35:DA:2613:U:H2'  | 2.44                     | 0.47              |
| 31:D6:11:LEU:HB3   | 31:D6:26:ASN:HD21 | 1.78                     | 0.47              |
| 35:DA:1416:G:O2'   | 35:DA:1417:C:H5   | 1.97                     | 0.47              |
| 35:DA:2086:U:H2'   | 35:DA:2087:G:C8   | 2.50                     | 0.47              |
| 22:CW:20:G:C5      | 35:DA:2169:A:H2   | 2.31                     | 0.47              |
| 35:DA:272(J):C:H5' | 35:DA:274:G:OP2   | 2.15                     | 0.47              |
| 35:DA:298:G:O5'    | 35:DA:298:G:H8    | 1.97                     | 0.47              |
| 35:DA:539:G:O2'    | 35:DA:540:C:H5'   | 2.14                     | 0.47              |
| 35:DA:753:C:H2'    | 35:DA:754:C:C6    | 2.49                     | 0.47              |
| 35:DA:769:G:H5'    | 35:DA:1379:A:N6   | 2.30                     | 0.47              |
| 35:DA:79:G:O2'     | 35:DA:80:G:H5'    | 2.14                     | 0.47              |
| 35:DA:915:C:H2'    | 35:DA:916:G:H8    | 1.79                     | 0.47              |
| 38:DD:161:THR:O    | 38:DD:162:SER:HB3 | 2.14                     | 0.47              |
| 39:DE:61:ARG:HG2   | 39:DE:62:PRO:CD   | 2.43                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:DF:10:PRO:HG2   | 40:DF:11:VAL:H    | 1.79                     | 0.47              |
| 40:DF:68:LYS:HG3   | 40:DF:69:HIS:HD2  | 1.79                     | 0.47              |
| 42:DH:13:LYS:C     | 42:DH:15:VAL:H    | 2.16                     | 0.47              |
| 42:DH:46:GLU:HG2   | 42:DH:46:GLU:H    | 1.35                     | 0.47              |
| 48:DP:33:ARG:O     | 48:DP:35:HIS:O    | 2.30                     | 0.47              |
| 51:DS:104:GLY:O    | 51:DS:106:ARG:N   | 2.46                     | 0.47              |
| 53:DU:59:ARG:HG2   | 53:DU:59:ARG:NH1  | 2.26                     | 0.47              |
| 55:DW:14:PRO:CG    | 55:DW:78:GLU:HB2  | 2.44                     | 0.47              |
| 58:DZ:116:VAL:HG12 | 58:DZ:117:LEU:N   | 2.30                     | 0.47              |
| 58:DZ:39:VAL:O     | 58:DZ:40:ASP:C    | 2.52                     | 0.47              |
| 1:AA:299:G:H2'     | 1:AA:300:A:H8     | 1.74                     | 0.47              |
| 1:AA:495:A:H4'     | 1:AA:496:A:OP1    | 2.14                     | 0.47              |
| 1:AA:965:A:C2      | 1:AA:969:A:C2     | 3.03                     | 0.47              |
| 5:AE:80:ILE:HD11   | 5:AE:138:ALA:HB1  | 1.97                     | 0.47              |
| 8:AH:26:VAL:HG23   | 8:AH:27:PRO:HD2   | 1.96                     | 0.47              |
| 8:AH:34:GLU:HB3    | 8:AH:118:VAL:HG21 | 1.96                     | 0.47              |
| 9:AI:9:ARG:HG2     | 9:AI:14:VAL:HA    | 1.96                     | 0.47              |
| 10:AJ:6:ILE:HG13   | 10:AJ:72:VAL:O    | 2.14                     | 0.47              |
| 11:AK:33:THR:HB    | 11:AK:38:ASN:O    | 2.14                     | 0.47              |
| 13:AM:66:LEU:CD1   | 13:AM:66:LEU:N    | 2.69                     | 0.47              |
| 17:AQ:60:ILE:HG22  | 17:AQ:72:ARG:O    | 2.15                     | 0.47              |
| 18:AR:53:ARG:C     | 18:AR:55:ARG:H    | 2.17                     | 0.47              |
| 22:AW:73:A:O2'     | 22:AW:74:A:O5'    | 2.27                     | 0.47              |
| 24:AY:106:VAL:CG2  | 24:AY:132:ARG:HG3 | 2.43                     | 0.47              |
| 61:AY:702:FUA:C20  | 61:AY:702:FUA:O1  | 2.62                     | 0.47              |
| 26:B1:90:ILE:O     | 26:B1:94:LEU:CD1  | 2.63                     | 0.47              |
| 30:B5:48:GLU:O     | 30:B5:49:CYS:HB3  | 2.13                     | 0.47              |
| 31:B6:7:ILE:HG22   | 31:B6:7:ILE:O     | 2.13                     | 0.47              |
| 35:BA:1100:C:H2'   | 35:BA:1100:C:O2   | 2.13                     | 0.47              |
| 35:BA:1263:U:H2'   | 35:BA:1264:G:C8   | 2.50                     | 0.47              |
| 35:BA:48:G:N2      | 35:BA:177:G:N2    | 2.62                     | 0.47              |
| 35:BA:1930:G:C2'   | 35:BA:1931:U:OP2  | 2.63                     | 0.47              |
| 35:BA:1985:G:O2'   | 35:BA:1986:A:H5'  | 2.13                     | 0.47              |
| 35:BA:2137:C:O2'   | 35:BA:2138:C:H5'  | 2.14                     | 0.47              |
| 35:BA:2309:A:C2'   | 35:BA:2310:A:H5'' | 2.44                     | 0.47              |
| 35:BA:2314:C:C2'   | 35:BA:2315:G:H5'  | 2.45                     | 0.47              |
| 35:BA:253:C:H2'    | 35:BA:254:G:O4'   | 2.15                     | 0.47              |
| 35:BA:2555:U:C2'   | 35:BA:2556:C:H5'  | 2.43                     | 0.47              |
| 35:BA:2564:A:OP1   | 35:BA:2648:C:H4'  | 2.14                     | 0.47              |
| 35:BA:2602:A:H4'   | 35:BA:2603:G:C5'  | 2.44                     | 0.47              |
| 35:BA:363:G:H2'    | 35:BA:363(A):A:H8 | 1.78                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:531:C:C5     | 35:BA:2035:G:C2    | 3.02                     | 0.47              |
| 35:BA:588:U:H1'    | 40:BF:90:PHE:HB3   | 1.96                     | 0.47              |
| 35:BA:783:A:H2'    | 35:BA:784:A:O5'    | 2.14                     | 0.47              |
| 37:BC:150:ILE:HG13 | 37:BC:154:ILE:HG13 | 1.96                     | 0.47              |
| 40:BF:127:GLU:O    | 40:BF:127:GLU:OE2  | 2.32                     | 0.47              |
| 40:BF:38:ARG:O     | 40:BF:42:ALA:CB    | 2.63                     | 0.47              |
| 41:BG:51:ARG:CZ    | 41:BG:53:LEU:HD21  | 2.44                     | 0.47              |
| 41:BG:77:ILE:HG22  | 41:BG:77:ILE:O     | 2.14                     | 0.47              |
| 43:BJ:69:UNK:O     | 43:BJ:70:UNK:C     | 2.62                     | 0.47              |
| 43:BJ:71:UNK:C     | 43:BJ:72:UNK:O     | 2.62                     | 0.47              |
| 49:BQ:12:GLN:HE21  | 49:BQ:72:LYS:HA    | 1.79                     | 0.47              |
| 49:BQ:87:LYS:CG    | 49:BQ:88:GLY:H     | 2.26                     | 0.47              |
| 52:BT:28:VAL:HG13  | 52:BT:46:GLU:CA    | 2.44                     | 0.47              |
| 52:BT:64:ARG:HG2   | 52:BT:64:ARG:NH1   | 2.29                     | 0.47              |
| 57:BY:54:LYS:HZ3   | 57:BY:55:TYR:HE2   | 1.63                     | 0.47              |
| 58:BZ:107:THR:HG23 | 58:BZ:111:VAL:HB   | 1.96                     | 0.47              |
| 1:CA:1221:G:P      | 19:CS:36:ARG:HD3   | 2.55                     | 0.47              |
| 1:CA:182:U:H5'     | 1:CA:183:G:P       | 2.54                     | 0.47              |
| 1:CA:417:C:H2'     | 1:CA:418:C:C6      | 2.50                     | 0.47              |
| 3:CC:165:THR:HG23  | 3:CC:165:THR:O     | 2.15                     | 0.47              |
| 3:CC:86:VAL:HG23   | 3:CC:87:LEU:HD23   | 1.96                     | 0.47              |
| 6:CF:50:TYR:CE1    | 18:CR:77:GLY:HA2   | 2.50                     | 0.47              |
| 16:CP:1:MET:HG3    | 16:CP:65:GLN:HG3   | 1.97                     | 0.47              |
| 16:CP:67:THR:HG22  | 16:CP:68:ASP:N     | 2.30                     | 0.47              |
| 6:CF:60:PHE:CE2    | 18:CR:78:LEU:HD21  | 2.50                     | 0.47              |
| 24:CY:637:ARG:HG3  | 24:CY:642:VAL:HG21 | 1.97                     | 0.47              |
| 26:D1:20:ARG:NH1   | 26:D1:20:ARG:HG2   | 2.29                     | 0.47              |
| 28:D3:56:VAL:CG1   | 28:D3:57:GLU:H     | 2.22                     | 0.47              |
| 31:D6:42:TRP:HA    | 31:D6:42:TRP:HE3   | 1.78                     | 0.47              |
| 35:DA:1053:C:H2'   | 35:DA:1054:A:C5'   | 2.41                     | 0.47              |
| 35:DA:1218:C:H2'   | 35:DA:1219:G:C8    | 2.50                     | 0.47              |
| 35:DA:1544:A:O2'   | 35:DA:1545:A:H5'   | 2.15                     | 0.47              |
| 35:DA:1658:C:O5'   | 35:DA:1658:C:H6    | 1.98                     | 0.47              |
| 35:DA:2373:G:O2'   | 35:DA:2374:C:H5'   | 2.14                     | 0.47              |
| 35:DA:2514:U:H2'   | 35:DA:2515:C:C6    | 2.39                     | 0.47              |
| 35:DA:253:C:H2'    | 35:DA:254:G:O4'    | 2.14                     | 0.47              |
| 35:DA:265:A:N6     | 35:DA:428:A:H1'    | 2.29                     | 0.47              |
| 35:DA:363:G:H2'    | 35:DA:363(A):A:H8  | 1.79                     | 0.47              |
| 35:DA:381:G:O2'    | 35:DA:382:G:H5'    | 2.14                     | 0.47              |
| 35:DA:383:U:H2'    | 35:DA:385:C:H5     | 1.79                     | 0.47              |
| 35:DA:41:C:H42     | 35:DA:437:G:H1     | 1.63                     | 0.47              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:DA:548:A:N3     | 35:DA:548:A:H2'   | 2.29                     | 0.47              |
| 35:DA:583:G:H2'    | 35:DA:584:C:H6    | 1.79                     | 0.47              |
| 35:DA:641:C:H2'    | 35:DA:642:G:O4'   | 2.15                     | 0.47              |
| 37:DC:202:PRO:HB2  | 37:DC:205:ALA:HB2 | 1.96                     | 0.47              |
| 38:DD:224:ALA:O    | 38:DD:225:ALA:HB2 | 2.15                     | 0.47              |
| 38:DD:44:ASN:OD1   | 38:DD:44:ASN:N    | 2.46                     | 0.47              |
| 39:DE:103:ASP:OD2  | 39:DE:201:THR:HA  | 2.15                     | 0.47              |
| 42:DH:94:TYR:HA    | 42:DH:106:THR:O   | 2.14                     | 0.47              |
| 42:DH:68:THR:C     | 42:DH:70:THR:N    | 2.68                     | 0.47              |
| 44:DK:69:THR:C     | 44:DK:70:LYS:HE3  | 2.35                     | 0.47              |
| 44:DK:93:ARG:HD2   | 44:DK:93:ARG:C    | 2.34                     | 0.47              |
| 46:DN:102:ALA:O    | 46:DN:106:MET:CE  | 2.62                     | 0.47              |
| 46:DN:2:LYS:HZ1    | 54:DV:12:TYR:HB3  | 1.80                     | 0.47              |
| 48:DP:102:ARG:HH21 | 48:DP:102:ARG:CB  | 2.27                     | 0.47              |
| 48:DP:67:MET:C     | 48:DP:68:GLN:HG3  | 2.35                     | 0.47              |
| 48:DP:95:VAL:HA    | 48:DP:99:LEU:CD2  | 2.40                     | 0.47              |
| 30:D5:44:THR:CG2   | 50:DR:101:ALA:N   | 2.78                     | 0.47              |
| 52:DT:55:ASN:ND2   | 52:DT:58:ASN:HD21 | 2.12                     | 0.47              |
| 52:DT:50:ILE:HA    | 52:DT:99:LEU:HD11 | 1.97                     | 0.47              |
| 54:DV:15:GLU:O     | 54:DV:16:PRO:C    | 2.53                     | 0.47              |
| 54:DV:35:LEU:C     | 54:DV:37:VAL:H    | 2.18                     | 0.47              |
| 54:DV:69:LYS:HE3   | 54:DV:71:LEU:HD21 | 1.97                     | 0.47              |
| 57:DY:58:GLY:O     | 57:DY:59:GLY:C    | 2.53                     | 0.47              |
| 1:AA:1125:U:H2'    | 1:AA:1126:U:H2'   | 1.97                     | 0.47              |
| 1:AA:1353:G:H2'    | 1:AA:1354:C:H6    | 1.80                     | 0.47              |
| 1:AA:1414:U:H2'    | 1:AA:1415:G:C8    | 2.49                     | 0.47              |
| 1:AA:1511:G:H2'    | 1:AA:1512:U:O4'   | 2.14                     | 0.47              |
| 1:AA:255:G:O3'     | 17:AQ:17:LYS:HD2  | 2.15                     | 0.47              |
| 1:AA:341:C:C2      | 1:AA:349:A:C2     | 3.03                     | 0.47              |
| 1:AA:824:C:H2'     | 1:AA:825:G:C8     | 2.46                     | 0.47              |
| 2:AB:164:VAL:CG1   | 2:AB:165:VAL:N    | 2.78                     | 0.47              |
| 3:AC:173:VAL:N     | 3:AC:174:PRO:HD3  | 2.29                     | 0.47              |
| 3:AC:59:ARG:HG2    | 3:AC:64:VAL:HA    | 1.95                     | 0.47              |
| 3:AC:86:VAL:HG23   | 3:AC:87:LEU:HD23  | 1.97                     | 0.47              |
| 8:AH:19:VAL:CG2    | 8:AH:21:LYS:HE2   | 2.44                     | 0.47              |
| 9:AI:114:TYR:HD1   | 10:AJ:60:ARG:HG3  | 1.79                     | 0.47              |
| 16:AP:54:GLU:OE2   | 16:AP:54:GLU:HA   | 2.13                     | 0.47              |
| 22:AV:73:A:O3'     | 22:AV:74:C:C6     | 2.68                     | 0.47              |
| 24:AY:277:VAL:HG13 | 24:AY:278:ASP:H   | 1.79                     | 0.47              |
| 24:AY:603:GLU:C    | 24:AY:676:TYR:HD1 | 2.18                     | 0.47              |
| 24:AY:87:HIS:NE2   | 24:AY:120:THR:OG1 | 2.47                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:B0:12:ASN:O    | 25:B0:14:ARG:N     | 2.41                     | 0.47              |
| 31:B6:16:CYS:O    | 31:B6:17:LYS:C     | 2.53                     | 0.47              |
| 34:B9:29:ASN:O    | 34:B9:31:LYS:N     | 2.47                     | 0.47              |
| 35:BA:1064:C:H42  | 35:BA:1074:G:H1    | 1.62                     | 0.47              |
| 35:BA:1260:G:H2'  | 35:BA:1261:C:C6    | 2.50                     | 0.47              |
| 35:BA:1683:C:H2'  | 35:BA:1684:C:H6    | 1.79                     | 0.47              |
| 35:BA:1771:C:H2'  | 35:BA:1772:G:C8    | 2.49                     | 0.47              |
| 35:BA:2163:C:H2'  | 35:BA:2164:C:H5'   | 1.96                     | 0.47              |
| 35:BA:2223:G:H2'  | 35:BA:2224:G:H5'   | 1.95                     | 0.47              |
| 35:BA:460:A:C2    | 35:BA:470:A:C4     | 3.03                     | 0.47              |
| 36:BB:40:U:O2'    | 36:BB:43:C:C5      | 2.67                     | 0.47              |
| 36:BB:54:G:H2'    | 36:BB:55:U:H6      | 1.80                     | 0.47              |
| 37:BC:29:LEU:O    | 37:BC:31:LYS:N     | 2.48                     | 0.47              |
| 37:BC:73:VAL:O    | 37:BC:73:VAL:HG13  | 2.15                     | 0.47              |
| 38:BD:28:GLU:HB2  | 38:BD:29:PRO:HD3   | 1.96                     | 0.47              |
| 39:BE:30:PRO:O    | 39:BE:32:PRO:HD3   | 2.14                     | 0.47              |
| 39:BE:76:ARG:O    | 39:BE:77:ILE:O     | 2.32                     | 0.47              |
| 39:BE:92:THR:OG1  | 39:BE:95:ILE:HD11  | 2.15                     | 0.47              |
| 40:BF:167:ALA:O   | 40:BF:169:ASN:N    | 2.48                     | 0.47              |
| 41:BG:106:LEU:O   | 41:BG:111:LEU:HD12 | 2.14                     | 0.47              |
| 48:BP:83:VAL:O    | 48:BP:83:VAL:HG13  | 2.14                     | 0.47              |
| 50:BR:3:HIS:O     | 50:BR:4:LEU:HB3    | 2.15                     | 0.47              |
| 54:BV:38:LEU:HD12 | 54:BV:56:SER:HA    | 1.95                     | 0.47              |
| 55:BW:41:LYS:C    | 55:BW:43:GLY:H     | 2.18                     | 0.47              |
| 1:CA:1281:U:H5'   | 1:CA:1282:C:OP2    | 2.15                     | 0.47              |
| 1:CA:337:C:H2'    | 1:CA:338:A:H8      | 1.79                     | 0.47              |
| 1:CA:830:G:O2'    | 1:CA:831:U:H5'     | 2.14                     | 0.47              |
| 2:CB:207:ALA:O    | 2:CB:208:ILE:C     | 2.53                     | 0.47              |
| 2:CB:53:ARG:O     | 2:CB:53:ARG:HG2    | 2.15                     | 0.47              |
| 7:CG:75:VAL:HG21  | 7:CG:144:MET:HB3   | 1.96                     | 0.47              |
| 9:CI:63:ILE:HG22  | 9:CI:64:THR:N      | 2.28                     | 0.47              |
| 10:CJ:5:ARG:HG3   | 10:CJ:71:LEU:HD11  | 1.96                     | 0.47              |
| 13:CM:79:LYS:HA   | 13:CM:82:MET:HG3   | 1.96                     | 0.47              |
| 17:CQ:45:HIS:HB2  | 17:CQ:65:ILE:HD13  | 1.97                     | 0.47              |
| 22:CW:52:C:C2'    | 22:CW:53:G:H5''    | 2.45                     | 0.47              |
| 24:CY:427:ALA:HB1 | 24:CY:466:LEU:HG   | 1.97                     | 0.47              |
| 26:D1:24:ALA:O    | 26:D1:27:GLU:O     | 2.33                     | 0.47              |
| 30:D5:58:LEU:HD13 | 30:D5:58:LEU:C     | 2.34                     | 0.47              |
| 30:D5:3:LYS:CD    | 30:D5:5:PRO:HD2    | 2.40                     | 0.47              |
| 31:D6:17:LYS:HB2  | 31:D6:44:ARG:NH1   | 2.27                     | 0.47              |
| 35:DA:585:G:H2'   | 35:DA:1251:C:H42   | 1.79                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:1534:U:H2'   | 35:DA:1535:A:O4'   | 2.13                     | 0.47              |
| 35:DA:191:A:O2'    | 35:DA:192:C:H5'    | 2.15                     | 0.47              |
| 30:D5:2:ALA:N      | 35:DA:2015:A:H1'   | 2.30                     | 0.47              |
| 35:DA:849:A:C8     | 35:DA:850:C:C5     | 3.02                     | 0.47              |
| 36:DB:20:C:C2'     | 36:DB:21:G:C5'     | 2.92                     | 0.47              |
| 40:DF:167:ALA:C    | 40:DF:170:LEU:HD23 | 2.35                     | 0.47              |
| 41:DG:111:LEU:HA   | 41:DG:114:ILE:HD11 | 1.96                     | 0.47              |
| 46:DN:15:LEU:CD2   | 46:DN:53:VAL:HB    | 2.45                     | 0.47              |
| 47:DO:107:ARG:HA   | 47:DO:112:MET:HE1  | 1.96                     | 0.47              |
| 48:DP:85:LEU:HA    | 48:DP:88:LEU:HB3   | 1.96                     | 0.47              |
| 49:DQ:17:LEU:C     | 49:DQ:18:LYS:HD2   | 2.35                     | 0.47              |
| 49:DQ:32:TYR:N     | 49:DQ:32:TYR:CD1   | 2.82                     | 0.47              |
| 49:DQ:12:GLN:HE21  | 49:DQ:72:LYS:HA    | 1.79                     | 0.47              |
| 51:DS:70:GLY:O     | 51:DS:72:ALA:N     | 2.48                     | 0.47              |
| 53:DU:39:LEU:O     | 53:DU:40:PHE:C     | 2.52                     | 0.47              |
| 54:DV:39:LEU:HA    | 54:DV:47:VAL:HG11  | 1.96                     | 0.47              |
| 35:DA:328:U:H4'    | 57:DY:68:HIS:NE2   | 2.29                     | 0.47              |
| 57:DY:13:VAL:CG2   | 57:DY:73:ARG:O     | 2.63                     | 0.47              |
| 58:DZ:176:PRO:O    | 58:DZ:177:PRO:O    | 2.32                     | 0.47              |
| 58:DZ:6:LYS:O      | 58:DZ:39:VAL:HG12  | 2.14                     | 0.47              |
| 58:DZ:79:ARG:O     | 58:DZ:80:ARG:CB    | 2.62                     | 0.47              |
| 58:DZ:9:TYR:CD1    | 58:DZ:35:ARG:NH2   | 2.77                     | 0.47              |
| 1:AA:184:G:O2'     | 1:AA:185:A:H5'     | 2.14                     | 0.47              |
| 1:AA:25:C:H2'      | 1:AA:26:A:C8       | 2.49                     | 0.47              |
| 2:AB:126:GLU:O     | 2:AB:127:ILE:C     | 2.53                     | 0.47              |
| 2:AB:77:ALA:O      | 2:AB:81:VAL:HG23   | 2.14                     | 0.47              |
| 5:AE:11:ILE:HD12   | 5:AE:31:LEU:HD13   | 1.96                     | 0.47              |
| 9:AI:95:LYS:NZ     | 9:AI:96:LEU:CD1    | 2.71                     | 0.47              |
| 14:AN:8:GLU:O      | 14:AN:11:LYS:HB2   | 2.14                     | 0.47              |
| 22:AV:59:A:H2'     | 22:AV:60:U:H5'     | 1.97                     | 0.47              |
| 24:AY:121:VAL:CG2  | 24:AY:122:TRP:N    | 2.77                     | 0.47              |
| 24:AY:139:MET:CE   | 24:AY:146:LEU:HB2  | 2.45                     | 0.47              |
| 24:AY:122:TRP:CE2  | 24:AY:157:LEU:HD12 | 2.49                     | 0.47              |
| 22:AV:36:U:O2      | 24:AY:502:GLY:HA2  | 2.15                     | 0.47              |
| 24:AY:514:VAL:HG21 | 24:AY:593:ALA:HB1  | 1.94                     | 0.47              |
| 24:AY:541:ALA:HB2  | 24:AY:579:GLU:HG3  | 1.96                     | 0.47              |
| 24:AY:601:ILE:O    | 24:AY:601:ILE:HG22 | 2.15                     | 0.47              |
| 30:B5:10:LYS:HB2   | 35:BA:2017:U:O2    | 2.14                     | 0.47              |
| 30:B5:11:THR:OG1   | 35:BA:1263:U:O3'   | 2.33                     | 0.47              |
| 30:B5:58:LEU:HD13  | 30:B5:58:LEU:C     | 2.35                     | 0.47              |
| 35:BA:112:U:C2'    | 35:BA:113:G:H5'    | 2.45                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:B5:19:ARG:NH1   | 35:BA:1266:G:OP1   | 2.46                     | 0.47              |
| 35:BA:1534:U:H2'   | 35:BA:1535:A:O4'   | 2.14                     | 0.47              |
| 35:BA:1783:A:C2    | 35:BA:2587:A:C4    | 3.01                     | 0.47              |
| 35:BA:1808:U:H2'   | 35:BA:1809:A:O4'   | 2.15                     | 0.47              |
| 35:BA:2148:G:O2'   | 35:BA:2149:G:H5'   | 2.14                     | 0.47              |
| 35:BA:2206:G:H21   | 35:BA:2207:G:H5'   | 1.78                     | 0.47              |
| 33:B8:42:ARG:HH11  | 35:BA:2350:C:H5    | 1.63                     | 0.47              |
| 35:BA:624:C:H41    | 48:BP:107:LYS:HZ2  | 1.61                     | 0.47              |
| 36:BB:95:C:O2'     | 36:BB:96:U:H5'     | 2.15                     | 0.47              |
| 38:BD:108:PRO:HB3  | 38:BD:143:HIS:CE1  | 2.50                     | 0.47              |
| 38:BD:55:GLY:O     | 38:BD:216:GLY:HA2  | 2.15                     | 0.47              |
| 38:BD:77:ALA:HB2   | 38:BD:97:TYR:CG    | 2.50                     | 0.47              |
| 41:BG:12:TYR:O     | 41:BG:16:ARG:HB2   | 2.14                     | 0.47              |
| 44:BK:112:MET:HE2  | 44:BK:120:LEU:HD21 | 1.95                     | 0.47              |
| 44:BK:98:ARG:HD2   | 44:BK:139:VAL:HG22 | 1.97                     | 0.47              |
| 46:BN:126:PRO:O    | 46:BN:127:ASP:CB   | 2.62                     | 0.47              |
| 53:BU:59:ARG:CG    | 53:BU:59:ARG:HH11  | 2.26                     | 0.47              |
| 53:BU:79:PHE:HE2   | 53:BU:83:LEU:HD11  | 1.80                     | 0.47              |
| 55:BW:107:LEU:HD22 | 55:BW:107:LEU:N    | 2.28                     | 0.47              |
| 57:BY:95:LYS:CE    | 57:BY:101:LYS:H    | 2.27                     | 0.47              |
| 58:BZ:27:VAL:N     | 58:BZ:37:VAL:HG22  | 2.29                     | 0.47              |
| 1:CA:1004:A:H5'    | 1:CA:1025:U:C4     | 2.50                     | 0.47              |
| 1:CA:1428:A:H2'    | 1:CA:1429:C:C6     | 2.49                     | 0.47              |
| 1:CA:473:G:H2'     | 1:CA:474:G:C8      | 2.46                     | 0.47              |
| 1:CA:475:G:O2'     | 1:CA:476:G:H5'     | 2.15                     | 0.47              |
| 1:CA:657:G:O2'     | 1:CA:658:G:H5'     | 2.14                     | 0.47              |
| 2:CB:126:GLU:O     | 2:CB:127:ILE:C     | 2.53                     | 0.47              |
| 2:CB:22:LYS:HE2    | 2:CB:22:LYS:CA     | 2.38                     | 0.47              |
| 2:CB:60:ASP:O      | 2:CB:64:ARG:NE     | 2.48                     | 0.47              |
| 4:CD:43:HIS:O      | 4:CD:45:GLN:N      | 2.48                     | 0.47              |
| 12:CL:86:ARG:HH22  | 12:CL:99:HIS:CD2   | 2.33                     | 0.47              |
| 15:CO:55:GLY:O     | 15:CO:56:LEU:C     | 2.53                     | 0.47              |
| 17:CQ:40:LYS:HD3   | 17:CQ:42:TYR:OH    | 2.15                     | 0.47              |
| 17:CQ:50:LYS:HG3   | 17:CQ:50:LYS:O     | 2.13                     | 0.47              |
| 20:CT:103:GLY:O    | 20:CT:104:LEU:C    | 2.52                     | 0.47              |
| 24:CY:343:ASN:ND2  | 24:CY:343:ASN:C    | 2.67                     | 0.47              |
| 24:CY:526:VAL:CG1  | 24:CY:566:THR:HG23 | 2.45                     | 0.47              |
| 28:D3:8:LEU:O      | 28:D3:31:LEU:HD22  | 2.15                     | 0.47              |
| 33:D8:4:MET:SD     | 33:D8:61:LEU:HD22  | 2.55                     | 0.47              |
| 35:DA:1582:C:O2'   | 35:DA:1583:A:H5'   | 2.15                     | 0.47              |
| 35:DA:1858:G:O2'   | 35:DA:1884:A:N6    | 2.48                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:2190:G:O2'   | 35:DA:2191:G:H5'   | 2.15                     | 0.47              |
| 35:DA:2579:C:O3'   | 39:DE:131:ALA:HB2  | 2.14                     | 0.47              |
| 35:DA:2886:G:H2'   | 35:DA:2887:U:C6    | 2.50                     | 0.47              |
| 35:DA:825:C:C2'    | 35:DA:826:U:H5'    | 2.45                     | 0.47              |
| 37:DC:11:LEU:C     | 37:DC:13:GLU:N     | 2.66                     | 0.47              |
| 38:DD:145:VAL:HG12 | 38:DD:146:GLU:O    | 2.15                     | 0.47              |
| 38:DD:145:VAL:CG1  | 38:DD:146:GLU:N    | 2.77                     | 0.47              |
| 39:DE:111:ARG:CZ   | 50:DR:2:ARG:NH2    | 2.78                     | 0.47              |
| 40:DF:167:ALA:O    | 40:DF:169:ASN:N    | 2.48                     | 0.47              |
| 40:DF:3:GLU:CB     | 40:DF:24:LEU:HG    | 2.43                     | 0.47              |
| 40:DF:74:ARG:O     | 40:DF:75:HIS:CG    | 2.68                     | 0.47              |
| 41:DG:121:ASN:CG   | 41:DG:124:SER:HB2  | 2.35                     | 0.47              |
| 41:DG:32:PRO:HB3   | 41:DG:163:ALA:HB2  | 1.97                     | 0.47              |
| 41:DG:53:LEU:N     | 41:DG:53:LEU:HD22  | 2.30                     | 0.47              |
| 41:DG:56:ALA:HA    | 41:DG:59:GLU:OE1   | 2.14                     | 0.47              |
| 42:DH:175:LYS:O    | 42:DH:176:ALA:HB2  | 2.13                     | 0.47              |
| 44:DK:18:THR:C     | 44:DK:20:ALA:H     | 2.18                     | 0.47              |
| 46:DN:40:PRO:HB3   | 53:DU:68:ALA:HB2   | 1.97                     | 0.47              |
| 46:DN:99:LEU:C     | 46:DN:99:LEU:HD13  | 2.35                     | 0.47              |
| 47:DO:60:ALA:CA    | 47:DO:87:ILE:HD11  | 2.44                     | 0.47              |
| 49:DQ:35:VAL:O     | 49:DQ:129:THR:HG22 | 2.14                     | 0.47              |
| 49:DQ:3:MET:HG3    | 49:DQ:4:PRO:O      | 2.13                     | 0.47              |
| 50:DR:65:LEU:O     | 50:DR:65:LEU:HD12  | 2.14                     | 0.47              |
| 51:DS:89:ARG:HG3   | 51:DS:92:TYR:N     | 2.30                     | 0.47              |
| 52:DT:48:ILE:HD12  | 52:DT:48:ILE:N     | 2.30                     | 0.47              |
| 52:DT:29:ARG:HG2   | 52:DT:85:LYS:HA    | 1.96                     | 0.47              |
| 55:DW:66:GLU:HA    | 55:DW:69:LEU:CD1   | 2.44                     | 0.47              |
| 57:DY:37:VAL:HG23  | 57:DY:38:ILE:N     | 2.30                     | 0.47              |
| 58:DZ:102:LEU:HD21 | 58:DZ:124:ILE:HD11 | 1.93                     | 0.47              |
| 58:DZ:16:SER:O     | 58:DZ:17:ALA:C     | 2.53                     | 0.47              |
| 1:AA:1231:G:C2'    | 1:AA:1232:U:H5'    | 2.45                     | 0.47              |
| 1:AA:201:C:C2'     | 1:AA:202:U:H5''    | 2.44                     | 0.47              |
| 1:AA:37:U:O2'      | 1:AA:500:G:H4'     | 2.15                     | 0.47              |
| 2:AB:126:GLU:O     | 2:AB:129:GLU:OE2   | 2.33                     | 0.47              |
| 4:AD:112:VAL:HG12  | 4:AD:116:GLN:OE1   | 2.13                     | 0.47              |
| 4:AD:22:LYS:O      | 4:AD:113:SER:HB3   | 2.15                     | 0.47              |
| 10:AJ:4:ILE:HB     | 10:AJ:74:ILE:HG13  | 1.96                     | 0.47              |
| 10:AJ:6:ILE:HG22   | 10:AJ:98:ILE:CD1   | 2.37                     | 0.47              |
| 11:AK:107:SER:C    | 11:AK:108:ILE:HD12 | 2.35                     | 0.47              |
| 12:AL:70:ILE:HG21  | 12:AL:77:LEU:HD12  | 1.96                     | 0.47              |
| 13:AM:63:THR:CG2   | 13:AM:64:TRP:H     | 2.24                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:AQ:51:TYR:CZ    | 17:AQ:73:VAL:HG11  | 2.50                     | 0.47              |
| 19:AS:6:LYS:CD     | 19:AS:6:LYS:H      | 2.28                     | 0.47              |
| 24:AY:432:ALA:HA   | 24:AY:438:PHE:CZ   | 2.50                     | 0.47              |
| 24:AY:495:GLY:O    | 24:AY:510:VAL:N    | 2.43                     | 0.47              |
| 26:B1:87:PRO:HG2   | 26:B1:88:LYS:H     | 1.80                     | 0.47              |
| 29:B4:50:VAL:O     | 29:B4:51:ASP:CB    | 2.62                     | 0.47              |
| 31:B6:11:LEU:HB3   | 31:B6:26:ASN:HD21  | 1.79                     | 0.47              |
| 31:B6:47:THR:CG2   | 31:B6:49:HIS:CE1   | 2.97                     | 0.47              |
| 35:BA:1052:C:P     | 35:BA:1052:C:O4'   | 2.73                     | 0.47              |
| 35:BA:1115:G:C8    | 35:BA:1115:G:H5'   | 2.47                     | 0.47              |
| 35:BA:112:U:H2'    | 35:BA:113:G:H5'    | 1.96                     | 0.47              |
| 35:BA:1436:G:H1'   | 35:BA:1477:A:O2'   | 2.15                     | 0.47              |
| 35:BA:1902:C:H4'   | 38:BD:244:ARG:CB   | 2.44                     | 0.47              |
| 26:B1:81:LYS:NZ    | 35:BA:271(H):G:O3' | 2.29                     | 0.47              |
| 35:BA:286:C:H2'    | 35:BA:287:C:H6     | 1.77                     | 0.47              |
| 35:BA:2888:C:H2'   | 35:BA:2889:C:C6    | 2.49                     | 0.47              |
| 35:BA:654(R):C:O2' | 35:BA:654(S):G:H8  | 1.98                     | 0.47              |
| 35:BA:733:G:O6     | 35:BA:761:A:C8     | 2.68                     | 0.47              |
| 35:BA:76:C:O2'     | 35:BA:77:C:H5'     | 2.14                     | 0.47              |
| 35:BA:775:G:O6     | 35:BA:787:U:H2'    | 2.14                     | 0.47              |
| 35:BA:946:G:H2'    | 35:BA:947:G:H8     | 1.80                     | 0.47              |
| 39:BE:119:ARG:HD2  | 39:BE:120:TRP:CE2  | 2.49                     | 0.47              |
| 39:BE:14:ILE:HD11  | 39:BE:173:VAL:HG11 | 1.96                     | 0.47              |
| 39:BE:174:ASP:OD2  | 39:BE:175:VAL:N    | 2.48                     | 0.47              |
| 39:BE:6:GLY:HA2    | 39:BE:27:LEU:O     | 2.15                     | 0.47              |
| 39:BE:38:THR:CG2   | 39:BE:40:GLU:HB2   | 2.45                     | 0.47              |
| 40:BF:185:ASP:HA   | 40:BF:188:ARG:HD3  | 1.95                     | 0.47              |
| 29:B4:26:SER:HB3   | 41:BG:105:LYS:NZ   | 2.30                     | 0.47              |
| 41:BG:110:ALA:O    | 41:BG:111:LEU:C    | 2.53                     | 0.47              |
| 42:BH:157:TYR:CE1  | 42:BH:171:LEU:HD21 | 2.23                     | 0.47              |
| 35:BA:1064:C:H5''  | 44:BK:86:LYS:HB2   | 1.97                     | 0.47              |
| 45:BL:89:UNK:O     | 45:BL:94:UNK:N     | 2.48                     | 0.47              |
| 49:BQ:24:GLY:CA    | 49:BQ:67:ARG:HH12  | 2.28                     | 0.47              |
| 52:BT:102:ILE:HB   | 52:BT:110:ILE:HD12 | 1.96                     | 0.47              |
| 54:BV:32:THR:HG22  | 54:BV:33:VAL:N     | 2.30                     | 0.47              |
| 53:BU:90:VAL:HG13  | 54:BV:39:LEU:HG    | 1.96                     | 0.47              |
| 56:BX:90:GLU:HA    | 56:BX:93:GLU:HG2   | 1.96                     | 0.47              |
| 57:BY:68:HIS:CB    | 57:BY:71:LYS:HZ3   | 2.27                     | 0.47              |
| 1:CA:1082:G:C2'    | 1:CA:1083:U:H5'    | 2.45                     | 0.47              |
| 1:CA:1123:A:H61    | 1:CA:1149:C:N4     | 2.13                     | 0.47              |
| 1:CA:189(A):C:H2'  | 1:CA:189(B):C:C6   | 2.49                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:189(C):C:H2' | 1:CA:189(D):C:O4'  | 2.15                     | 0.47              |
| 1:CA:470:C:C2'    | 1:CA:471:G:OP1     | 2.63                     | 0.47              |
| 1:CA:631:G:C2'    | 1:CA:632:A:C8      | 2.94                     | 0.47              |
| 1:CA:636:U:H2'    | 1:CA:637:G:H8      | 1.80                     | 0.47              |
| 2:CB:77:ALA:HA    | 2:CB:80:ILE:HD13   | 1.96                     | 0.47              |
| 3:CC:151:VAL:CG1  | 3:CC:152:ILE:N     | 2.77                     | 0.47              |
| 6:CF:21:LEU:O     | 6:CF:24:GLU:HB3    | 2.14                     | 0.47              |
| 7:CG:18:TYR:HD2   | 7:CG:59:LEU:HD13   | 1.79                     | 0.47              |
| 13:CM:37:THR:HG21 | 13:CM:56:LEU:HA    | 1.96                     | 0.47              |
| 14:CN:8:GLU:O     | 14:CN:11:LYS:HB2   | 2.15                     | 0.47              |
| 1:CA:452:A:H4'    | 16:CP:72:ARG:CZ    | 2.44                     | 0.47              |
| 18:CR:66:LEU:HG   | 18:CR:70:ILE:CD1   | 2.44                     | 0.47              |
| 22:CW:62:C:O2'    | 22:CW:63:C:H5'     | 2.14                     | 0.47              |
| 24:CY:290:LYS:HB3 | 24:CY:298:VAL:CG2  | 2.44                     | 0.47              |
| 24:CY:346:LYS:NZ  | 24:CY:384:ILE:HD11 | 2.29                     | 0.47              |
| 24:CY:421:GLN:O   | 24:CY:424:LEU:HB3  | 2.15                     | 0.47              |
| 29:D4:14:ILE:O    | 29:D4:15:ILE:HD13  | 2.15                     | 0.47              |
| 29:D4:12:ALA:HB2  | 29:D4:29:PRO:HA    | 1.97                     | 0.47              |
| 34:D9:16:VAL:HA   | 34:D9:25:VAL:HG22  | 1.97                     | 0.47              |
| 35:DA:1378:A:HO2' | 35:DA:1379:A:H5''  | 1.72                     | 0.47              |
| 35:DA:1774:C:O5'  | 35:DA:1774:C:H6    | 1.97                     | 0.47              |
| 35:DA:2199:A:H3'  | 35:DA:2200:C:C6    | 2.48                     | 0.47              |
| 35:DA:2476:A:C2   | 35:DA:2477:C:C6    | 3.03                     | 0.47              |
| 35:DA:2745:C:C4   | 35:DA:2746:U:C4    | 3.03                     | 0.47              |
| 35:DA:325:G:O2'   | 35:DA:326:G:H5'    | 2.14                     | 0.47              |
| 35:DA:654(S):G:C5 | 35:DA:654(T):C:H1' | 2.50                     | 0.47              |
| 35:DA:754:C:H2'   | 35:DA:755:C:C6     | 2.50                     | 0.47              |
| 35:DA:925:C:C4    | 35:DA:926:A:N7     | 2.83                     | 0.47              |
| 37:DC:156:GLU:OE1 | 37:DC:161:ARG:HD3  | 2.15                     | 0.47              |
| 35:DA:2203:U:H1'  | 38:DD:151:LYS:HE3  | 1.97                     | 0.47              |
| 38:DD:99:ASP:C    | 38:DD:99:ASP:OD2   | 2.53                     | 0.47              |
| 41:DG:46:ALA:HA   | 41:DG:51:ARG:HB2   | 1.97                     | 0.47              |
| 46:DN:134:ARG:HG3 | 46:DN:134:ARG:O    | 2.15                     | 0.47              |
| 46:DN:45:ASN:N    | 46:DN:45:ASN:ND2   | 2.56                     | 0.47              |
| 50:DR:118:GLU:HA  | 50:DR:118:GLU:OE1  | 2.15                     | 0.47              |
| 51:DS:33:LYS:HG2  | 51:DS:34:HIS:CD2   | 2.49                     | 0.47              |
| 35:DA:1155:A:O3'  | 53:DU:55:ARG:NH1   | 2.48                     | 0.47              |
| 54:DV:19:LYS:HE2  | 54:DV:19:LYS:HA    | 1.96                     | 0.47              |
| 1:AA:1115:C:H2'   | 1:AA:1116:C:H6     | 1.79                     | 0.47              |
| 1:AA:720:C:H6     | 1:AA:720:C:O5'     | 1.98                     | 0.47              |
| 1:AA:98:G:H2'     | 1:AA:99:U:O4'      | 2.15                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 4:AD:18:LYS:O      | 4:AD:19:LEU:HD12    | 2.15                     | 0.47              |
| 7:AG:65:ALA:HA     | 7:AG:128:ALA:HA     | 1.96                     | 0.47              |
| 9:AI:118:LYS:O     | 9:AI:119:ALA:HB3    | 2.14                     | 0.47              |
| 10:AJ:4:ILE:HB     | 10:AJ:74:ILE:CD1    | 2.45                     | 0.47              |
| 12:AL:59:ARG:CZ    | 24:AY:422:GLU:OE2   | 2.62                     | 0.47              |
| 12:AL:33:ARG:HG3   | 12:AL:60:LEU:HD12   | 1.96                     | 0.47              |
| 14:AN:41:ARG:CG    | 14:AN:41:ARG:NH1    | 2.78                     | 0.47              |
| 15:AO:74:ASP:C     | 15:AO:76:GLU:N      | 2.69                     | 0.47              |
| 20:AT:74:LYS:HB2   | 20:AT:75:ASN:H      | 1.47                     | 0.47              |
| 24:AY:17:ILE:HG22  | 24:AY:25:LYS:HG2    | 1.96                     | 0.47              |
| 24:AY:202:PRO:O    | 24:AY:203:GLU:C     | 2.53                     | 0.47              |
| 24:AY:357:ARG:HH11 | 24:AY:373:ASP:CG    | 2.19                     | 0.47              |
| 24:AY:346:LYS:HE2  | 24:AY:384:ILE:HG12  | 1.97                     | 0.47              |
| 25:B0:55:ARG:HB3   | 25:B0:55:ARG:HE     | 1.46                     | 0.47              |
| 30:B5:56:LYS:O     | 30:B5:57:VAL:O      | 2.32                     | 0.47              |
| 31:B6:15:GLU:N     | 31:B6:49:HIS:CD2    | 2.83                     | 0.47              |
| 31:B6:6:ARG:C      | 31:B6:7:ILE:CD1     | 2.83                     | 0.47              |
| 33:B8:55:ALA:O     | 33:B8:59:LYS:HE2    | 2.15                     | 0.47              |
| 34:B9:17:ILE:HG22  | 34:B9:18:ARG:H      | 1.80                     | 0.47              |
| 35:BA:1132:A:H2'   | 35:BA:1133:U:H6     | 1.80                     | 0.47              |
| 35:BA:769:G:H4'    | 35:BA:1379:A:N1     | 2.30                     | 0.47              |
| 35:BA:1539:G:N3    | 35:BA:1540:U:H1'    | 2.29                     | 0.47              |
| 35:BA:1805:U:H2'   | 35:BA:1806:C:H6     | 1.79                     | 0.47              |
| 35:BA:1948:G:C5'   | 35:BA:1948:G:H8     | 2.28                     | 0.47              |
| 35:BA:2223:G:C2'   | 35:BA:2224:G:H5'    | 2.44                     | 0.47              |
| 35:BA:272(H):C:C2' | 35:BA:272(I):U:H5'' | 2.42                     | 0.47              |
| 35:BA:363(F):A:H1' | 35:BA:364:C:H5      | 1.79                     | 0.47              |
| 35:BA:548:A:H2'    | 35:BA:548:A:N3      | 2.29                     | 0.47              |
| 38:BD:155:LEU:N    | 38:BD:155:LEU:CD1   | 2.77                     | 0.47              |
| 39:BE:107:THR:HA   | 39:BE:163:GLU:O     | 2.15                     | 0.47              |
| 39:BE:37:ARG:HA    | 39:BE:42:ASP:OD2    | 2.15                     | 0.47              |
| 42:BH:154:PRO:C    | 42:BH:156:ALA:H     | 2.18                     | 0.47              |
| 46:BN:131:GLN:NE2  | 46:BN:133:GLN:N     | 2.63                     | 0.47              |
| 46:BN:15:LEU:HB2   | 46:BN:134:ARG:HB2   | 1.97                     | 0.47              |
| 46:BN:2:LYS:HZ1    | 54:BV:12:TYR:HB3    | 1.79                     | 0.47              |
| 48:BP:112:LEU:HD22 | 48:BP:113:LYS:N     | 2.29                     | 0.47              |
| 48:BP:32:THR:HG22  | 48:BP:37:GLY:HA2    | 1.97                     | 0.47              |
| 52:BT:50:ILE:HA    | 52:BT:99:LEU:HD11   | 1.96                     | 0.47              |
| 53:BU:97:ASP:C     | 53:BU:99:ALA:H      | 2.19                     | 0.47              |
| 54:BV:2:PHE:HB3    | 54:BV:41:GLY:C      | 2.34                     | 0.47              |
| 54:BV:39:LEU:HA    | 54:BV:47:VAL:HG11   | 1.95                     | 0.47              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 57:BY:105:ALA:O   | 57:BY:106:LEU:HB2  | 2.15                     | 0.47              |
| 58:BZ:121:HIS:CD2 | 58:BZ:123:ASP:O    | 2.68                     | 0.47              |
| 58:BZ:96:VAL:HG22 | 58:BZ:97:GLU:N     | 2.30                     | 0.47              |
| 1:CA:1209:C:O2'   | 1:CA:1210:C:H5'    | 2.15                     | 0.47              |
| 1:CA:203:U:H5'    | 1:CA:216:G:N2      | 2.30                     | 0.47              |
| 1:CA:142:G:H1     | 1:CA:221:C:H42     | 1.63                     | 0.47              |
| 3:CC:131:ARG:HH22 | 3:CC:168:ALA:HB2   | 1.78                     | 0.47              |
| 3:CC:72:LYS:HE3   | 3:CC:72:LYS:CA     | 2.45                     | 0.47              |
| 4:CD:74:GLN:HA    | 4:CD:77:ASN:HD22   | 1.79                     | 0.47              |
| 5:CE:144:THR:O    | 5:CE:146:ALA:N     | 2.48                     | 0.47              |
| 6:CF:91:VAL:CG1   | 6:CF:92:LYS:N      | 2.77                     | 0.47              |
| 12:CL:41:ARG:NH1  | 12:CL:41:ARG:CB    | 2.78                     | 0.47              |
| 22:CW:14:A:C4     | 22:CW:23:G:N2      | 2.83                     | 0.47              |
| 24:CY:11:ARG:C    | 24:CY:12:LEU:HD22  | 2.36                     | 0.47              |
| 24:CY:226:ASN:C   | 24:CY:228:MET:N    | 2.67                     | 0.47              |
| 24:CY:314:PHE:CZ  | 24:CY:327:PHE:HB3  | 2.50                     | 0.47              |
| 24:CY:454:MET:N   | 24:CY:458:HIS:HD2  | 2.12                     | 0.47              |
| 24:CY:632:LEU:CD1 | 24:CY:645:ALA:HA   | 2.44                     | 0.47              |
| 61:CY:702:FUA:C31 | 61:CY:702:FUA:O4   | 2.62                     | 0.47              |
| 27:D2:61:LEU:HD12 | 35:DA:72:U:H6      | 1.77                     | 0.47              |
| 28:D3:7:LYS:HE3   | 28:D3:32:GLN:O     | 2.15                     | 0.47              |
| 35:DA:1241:A:H2'  | 35:DA:1242:A:O4'   | 2.15                     | 0.47              |
| 35:DA:1336:A:O2'  | 35:DA:1337:G:H5'   | 2.15                     | 0.47              |
| 35:DA:2056:G:N2   | 35:DA:2057:A:N9    | 2.63                     | 0.47              |
| 33:D8:28:GLY:H    | 35:DA:2393:A:P     | 2.37                     | 0.47              |
| 35:DA:2704:C:H2'  | 35:DA:2705:A:O4'   | 2.15                     | 0.47              |
| 35:DA:2759:G:O2'  | 35:DA:2760:C:H5'   | 2.14                     | 0.47              |
| 35:DA:2762:G:H8   | 35:DA:2762:G:C5'   | 2.26                     | 0.47              |
| 35:DA:706:A:H2'   | 35:DA:707:G:O4'    | 2.15                     | 0.47              |
| 36:DB:51:G:H5'    | 36:DB:52:A:OP2     | 2.15                     | 0.47              |
| 35:DA:2170:A:H5'' | 37:DC:135:ARG:HE   | 1.80                     | 0.47              |
| 37:DC:150:ILE:O   | 37:DC:154:ILE:HG13 | 2.15                     | 0.47              |
| 35:DA:2787:C:O2   | 39:DE:61:ARG:HD3   | 2.15                     | 0.47              |
| 40:DF:157:VAL:O   | 40:DF:157:VAL:HG23 | 2.15                     | 0.47              |
| 40:DF:36:VAL:O    | 40:DF:39:TRP:HB3   | 2.15                     | 0.47              |
| 42:DH:138:LYS:C   | 42:DH:140:LYS:N    | 2.67                     | 0.47              |
| 43:DJ:8:UNK:C     | 43:DJ:10:UNK:N     | 2.78                     | 0.47              |
| 43:DJ:95:UNK:C    | 43:DJ:97:UNK:N     | 2.78                     | 0.47              |
| 44:DK:2:LYS:HB2   | 44:DK:2:LYS:NZ     | 2.30                     | 0.47              |
| 44:DK:30:HIS:CG   | 44:DK:59:ILE:HB    | 2.50                     | 0.47              |
| 46:DN:14:VAL:HG11 | 46:DN:137:LYS:CD   | 2.45                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:DO:22:ILE:O     | 47:DO:23:ARG:HB3   | 2.14                     | 0.47              |
| 48:DP:99:LEU:HG    | 48:DP:100:LEU:HD22 | 1.96                     | 0.47              |
| 51:DS:14:VAL:CG1   | 51:DS:16:ASN:HD22  | 2.28                     | 0.47              |
| 52:DT:30:VAL:HG21  | 52:DT:83:ILE:CG1   | 2.44                     | 0.47              |
| 56:DX:28:PHE:CD1   | 56:DX:28:PHE:N     | 2.83                     | 0.47              |
| 56:DX:7:VAL:HB     | 56:DX:8:ILE:HD12   | 1.96                     | 0.47              |
| 58:DZ:163:LEU:CD2  | 58:DZ:163:LEU:H    | 2.24                     | 0.47              |
| 1:AA:1010:G:C6     | 1:AA:1020:U:H1'    | 2.50                     | 0.47              |
| 1:AA:1220:G:H2'    | 1:AA:1221:G:C8     | 2.47                     | 0.47              |
| 1:AA:1313:U:P      | 19:AS:6:LYS:HG3    | 2.55                     | 0.47              |
| 1:AA:1347:G:C2'    | 1:AA:1348:U:OP2    | 2.63                     | 0.47              |
| 1:AA:1440:C:H2'    | 1:AA:1441:G:H5'    | 1.96                     | 0.47              |
| 1:AA:1485:U:O2'    | 1:AA:1486:G:H5'    | 2.15                     | 0.47              |
| 1:AA:337:C:H2'     | 1:AA:338:A:H8      | 1.79                     | 0.47              |
| 1:AA:738:C:H2'     | 1:AA:739:C:H6      | 1.80                     | 0.47              |
| 2:AB:77:ALA:HA     | 2:AB:80:ILE:HD13   | 1.96                     | 0.47              |
| 3:AC:112:SER:OG    | 3:AC:114:PRO:HD2   | 2.15                     | 0.47              |
| 3:AC:69:HIS:HA     | 3:AC:104:GLN:HB2   | 1.97                     | 0.47              |
| 4:AD:133:VAL:HG12  | 4:AD:134:ASP:N     | 2.30                     | 0.47              |
| 10:AJ:50:ILE:N     | 10:AJ:50:ILE:HD13  | 2.16                     | 0.47              |
| 10:AJ:61:GLU:HG3   | 14:AN:58:LYS:HZ3   | 1.80                     | 0.47              |
| 10:AJ:63:PHE:HB3   | 14:AN:58:LYS:CA    | 2.41                     | 0.47              |
| 16:AP:67:THR:N     | 16:AP:70:ALA:HB3   | 2.30                     | 0.47              |
| 18:AR:31:LEU:N     | 18:AR:31:LEU:HD23  | 2.23                     | 0.47              |
| 18:AR:79:LEU:HD22  | 18:AR:80:PRO:HD2   | 1.97                     | 0.47              |
| 13:AM:86:CYS:HA    | 19:AS:73:GLU:O     | 2.15                     | 0.47              |
| 20:AT:33:ILE:HG21  | 20:AT:63:ILE:HG12  | 1.97                     | 0.47              |
| 24:AY:139:MET:HG3  | 24:AY:260:LEU:HB2  | 1.97                     | 0.47              |
| 24:AY:359:HIS:C    | 24:AY:361:ASN:H    | 2.18                     | 0.47              |
| 24:AY:409:ILE:HG22 | 24:AY:459:LEU:HD13 | 1.97                     | 0.47              |
| 24:AY:635:GLU:HA   | 24:AY:636:PRO:HD2  | 1.74                     | 0.47              |
| 24:AY:119:GLU:OE1  | 24:AY:666:ARG:HG2  | 2.15                     | 0.47              |
| 28:B3:7:LYS:HE3    | 28:B3:32:GLN:O     | 2.15                     | 0.47              |
| 28:B3:46:ASN:O     | 28:B3:49:LYS:N     | 2.47                     | 0.47              |
| 31:B6:11:LEU:HD12  | 31:B6:25:LYS:HA    | 1.97                     | 0.47              |
| 33:B8:51:ALA:HA    | 33:B8:54:GLU:CD    | 2.35                     | 0.47              |
| 33:B8:6:THR:HG21   | 33:B8:63:PRO:HD3   | 1.95                     | 0.47              |
| 35:BA:1022:G:O2'   | 35:BA:1023:U:P     | 2.72                     | 0.47              |
| 35:BA:1416:G:O2'   | 35:BA:1417:C:H5    | 1.98                     | 0.47              |
| 35:BA:1491:G:O2'   | 38:BD:101:GLU:HB2  | 2.14                     | 0.47              |
| 35:BA:154(A):C:H42 | 35:BA:172:C:N4     | 2.13                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:2415:G:H2'   | 35:BA:2416:C:C6    | 2.50                     | 0.47              |
| 35:BA:2453:A:H2'   | 35:BA:2454:G:C8    | 2.48                     | 0.47              |
| 35:BA:2464:C:O2'   | 35:BA:2465:C:H6    | 1.97                     | 0.47              |
| 35:BA:2551:C:H2'   | 35:BA:2552:U:C6    | 2.51                     | 0.47              |
| 35:BA:2552:U:C2    | 35:BA:2554:U:C5'   | 2.97                     | 0.47              |
| 35:BA:2762:G:H2'   | 35:BA:2763:G:H5'   | 1.97                     | 0.47              |
| 35:BA:325:G:H2'    | 35:BA:326:G:H8     | 1.80                     | 0.47              |
| 35:BA:519:U:O2'    | 35:BA:520:G:H5'    | 2.15                     | 0.47              |
| 35:BA:894:C:C2'    | 35:BA:895:U:H5'    | 2.45                     | 0.47              |
| 37:BC:29:LEU:CD2   | 37:BC:29:LEU:C     | 2.83                     | 0.47              |
| 38:BD:117:VAL:CG2  | 38:BD:118:VAL:N    | 2.78                     | 0.47              |
| 40:BF:176:LEU:HD11 | 40:BF:180:GLY:HA3  | 1.97                     | 0.47              |
| 40:BF:205:ARG:O    | 40:BF:206:ILE:HD13 | 2.15                     | 0.47              |
| 13:AM:61:GLU:OE2   | 41:BG:113:ARG:NH2  | 2.46                     | 0.47              |
| 41:BG:157:ILE:CG2  | 41:BG:158:ALA:N    | 2.78                     | 0.47              |
| 41:BG:29:TRP:O     | 41:BG:31:VAL:N     | 2.48                     | 0.47              |
| 41:BG:75:LYS:C     | 41:BG:76:SER:HG    | 2.15                     | 0.47              |
| 42:BH:13:LYS:O     | 42:BH:15:VAL:N     | 2.37                     | 0.47              |
| 42:BH:70:THR:HG22  | 42:BH:74:ASN:ND2   | 2.30                     | 0.47              |
| 42:BH:89:ILE:HD12  | 42:BH:89:ILE:C     | 2.36                     | 0.47              |
| 44:BK:108:ALA:O    | 44:BK:112:MET:HB3  | 2.15                     | 0.47              |
| 44:BK:30:HIS:CG    | 44:BK:59:ILE:HB    | 2.50                     | 0.47              |
| 46:BN:65:LYS:CB    | 46:BN:69:GLN:HG3   | 2.42                     | 0.47              |
| 48:BP:112:LEU:H    | 48:BP:128:HIS:HD2  | 1.61                     | 0.47              |
| 49:BQ:59:ARG:O     | 49:BQ:60:ARG:HB2   | 2.15                     | 0.47              |
| 50:BR:26:LYS:HE2   | 50:BR:71:GLN:H     | 1.79                     | 0.47              |
| 51:BS:25:ARG:CG    | 51:BS:26:LEU:N     | 2.78                     | 0.47              |
| 51:BS:42:ASP:O     | 51:BS:43:GLU:HB2   | 2.14                     | 0.47              |
| 52:BT:7:ILE:O      | 52:BT:10:VAL:HB    | 2.14                     | 0.47              |
| 57:BY:58:GLY:O     | 57:BY:59:GLY:C     | 2.54                     | 0.47              |
| 1:CA:1253:G:C2     | 1:CA:1254:C:C2     | 3.02                     | 0.47              |
| 1:CA:1321:C:C5'    | 1:CA:1322:C:C5'    | 2.93                     | 0.47              |
| 1:CA:1422:G:H2'    | 1:CA:1423:G:C8     | 2.50                     | 0.47              |
| 1:CA:1490:C:C6     | 1:CA:1490:C:C5'    | 2.92                     | 0.47              |
| 1:CA:355:C:C4      | 1:CA:356:A:N7      | 2.83                     | 0.47              |
| 1:CA:509:A:H3'     | 1:CA:510:A:C8      | 2.50                     | 0.47              |
| 1:CA:720:C:H6      | 1:CA:720:C:O5'     | 1.98                     | 0.47              |
| 1:CA:830:G:H2'     | 1:CA:831:U:C6      | 2.50                     | 0.47              |
| 1:CA:836:G:C6      | 1:CA:851:G:C6      | 3.03                     | 0.47              |
| 4:CD:112:VAL:HG12  | 4:CD:116:GLN:OE1   | 2.14                     | 0.47              |
| 8:CH:29:SER:OG     | 8:CH:32:LYS:HG3    | 2.15                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:CI:5:TYR:CG      | 9:CI:6:GLY:N       | 2.83                     | 0.47              |
| 10:CJ:90:LEU:H     | 10:CJ:91:PRO:HD3   | 1.80                     | 0.47              |
| 18:CR:26:LEU:HD21  | 18:CR:42:ARG:NH1   | 2.30                     | 0.47              |
| 19:CS:48:THR:HG22  | 19:CS:61:TYR:HD1   | 1.80                     | 0.47              |
| 19:CS:6:LYS:HE3    | 19:CS:6:LYS:N      | 2.29                     | 0.47              |
| 20:CT:11:SER:HA    | 20:CT:13:LEU:CD1   | 2.44                     | 0.47              |
| 7:CG:82:GLY:HA3    | 23:CX:13:A:C2      | 2.48                     | 0.47              |
| 24:CY:237:PRO:HB2  | 24:CY:242:LEU:HG   | 1.97                     | 0.47              |
| 24:CY:459:LEU:HD12 | 24:CY:460:GLU:H    | 1.80                     | 0.47              |
| 24:CY:457:LEU:O    | 24:CY:460:GLU:N    | 2.48                     | 0.47              |
| 24:CY:515:GLU:HG3  | 24:CY:564:LYS:HB3  | 1.97                     | 0.47              |
| 24:CY:615:GLU:OE2  | 24:CY:666:ARG:NH2  | 2.48                     | 0.47              |
| 26:D1:44:PRO:O     | 35:DA:2230:G:H4'   | 2.15                     | 0.47              |
| 26:D1:4:VAL:HG22   | 26:D1:5:CYS:N      | 2.30                     | 0.47              |
| 28:D3:43:ILE:O     | 28:D3:47:VAL:HG23  | 2.15                     | 0.47              |
| 31:D6:33:LYS:HG2   | 31:D6:34:LEU:H     | 1.80                     | 0.47              |
| 35:DA:1034:G:OP1   | 35:DA:1034:G:H8    | 1.98                     | 0.47              |
| 35:DA:1582:C:O2'   | 35:DA:1586:A:C8    | 2.66                     | 0.47              |
| 35:DA:1688:U:O2    | 35:DA:1700:A:H5''  | 2.15                     | 0.47              |
| 35:DA:2483:C:H5'   | 35:DA:2484:G:OP2   | 2.15                     | 0.47              |
| 35:DA:2543:G:H2'   | 35:DA:2544:G:C8    | 2.50                     | 0.47              |
| 35:DA:2839:G:H2'   | 35:DA:2840:C:H6    | 1.79                     | 0.47              |
| 35:DA:834:C:O2'    | 35:DA:835:A:H5'    | 2.15                     | 0.47              |
| 37:DC:34:ALA:CB    | 37:DC:179:ALA:HB2  | 2.44                     | 0.47              |
| 38:DD:34:VAL:O     | 38:DD:36:PRO:HG2   | 2.15                     | 0.47              |
| 38:DD:55:GLY:O     | 38:DD:216:GLY:HA2  | 2.15                     | 0.47              |
| 39:DE:36:ARG:NH2   | 39:DE:88:GLY:N     | 2.61                     | 0.47              |
| 39:DE:69:LYS:HD3   | 39:DE:89:ASP:HA    | 1.97                     | 0.47              |
| 41:DG:82:LEU:HD22  | 41:DG:87:PRO:HB3   | 1.96                     | 0.47              |
| 46:DN:131:GLN:NE2  | 46:DN:133:GLN:N    | 2.62                     | 0.47              |
| 46:DN:16:ILE:O     | 46:DN:54:VAL:HA    | 2.15                     | 0.47              |
| 49:DQ:62:GLY:O     | 58:DZ:178:GLU:OE1  | 2.32                     | 0.47              |
| 51:DS:104:GLY:C    | 51:DS:106:ARG:N    | 2.66                     | 0.47              |
| 52:DT:128:GLU:O    | 52:DT:129:ARG:HD3  | 2.15                     | 0.47              |
| 52:DT:134:GLU:O    | 52:DT:135:ALA:CB   | 2.62                     | 0.47              |
| 53:DU:110:VAL:HG12 | 53:DU:114:LYS:HD2  | 1.93                     | 0.47              |
| 53:DU:97:ASP:C     | 53:DU:99:ALA:H     | 2.18                     | 0.47              |
| 57:DY:31:LEU:HD22  | 57:DY:31:LEU:H     | 1.77                     | 0.47              |
| 58:DZ:153:SER:HB2  | 58:DZ:163:LEU:HD11 | 1.95                     | 0.47              |
| 1:AA:1010:G:N1     | 1:AA:1020:U:H1'    | 2.30                     | 0.46              |
| 1:AA:1064:G:H21    | 1:AA:1190:G:H2'    | 1.78                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1440:C:C2'    | 1:AA:1441:G:H5'    | 2.46                     | 0.46              |
| 1:AA:1458:G:C6     | 1:AA:1459:C:C4     | 3.03                     | 0.46              |
| 1:AA:738:C:H5''    | 6:AF:69:GLU:HB2    | 1.95                     | 0.46              |
| 1:AA:8:A:C6        | 4:AD:209:ARG:HB2   | 2.50                     | 0.46              |
| 2:AB:86:GLU:C      | 2:AB:88:ALA:N      | 2.68                     | 0.46              |
| 3:AC:78:GLY:HA3    | 3:AC:83:ARG:HB3    | 1.96                     | 0.46              |
| 5:AE:144:THR:O     | 5:AE:145:LYS:C     | 2.53                     | 0.46              |
| 5:AE:53:LEU:O      | 5:AE:56:GLN:HB3    | 2.15                     | 0.46              |
| 5:AE:72:GLN:O      | 5:AE:73:ASN:HB2    | 2.15                     | 0.46              |
| 7:AG:75:VAL:HG21   | 7:AG:144:MET:HB3   | 1.97                     | 0.46              |
| 7:AG:92:SER:O      | 7:AG:93:PRO:C      | 2.52                     | 0.46              |
| 9:AI:10:ARG:CZ     | 9:AI:105:ASP:OD2   | 2.63                     | 0.46              |
| 13:AM:22:ILE:HD12  | 13:AM:22:ILE:N     | 2.30                     | 0.46              |
| 13:AM:45:VAL:HA    | 13:AM:48:LEU:CD1   | 2.45                     | 0.46              |
| 10:AJ:61:GLU:HG3   | 14:AN:58:LYS:CE    | 2.45                     | 0.46              |
| 19:AS:5:LEU:HG     | 19:AS:10:PHE:HD1   | 1.80                     | 0.46              |
| 22:AW:51:U:H3      | 22:AW:65:G:H1      | 1.63                     | 0.46              |
| 24:AY:182:ARG:HH11 | 24:AY:182:ARG:HG3  | 1.80                     | 0.46              |
| 24:AY:289:ILE:CD1  | 24:AY:331:TYR:CZ   | 2.97                     | 0.46              |
| 24:AY:74:TRP:NE1   | 24:AY:273:LEU:HB3  | 2.30                     | 0.46              |
| 30:B5:51:TYR:HD2   | 30:B5:52:TYR:H     | 1.62                     | 0.46              |
| 32:B7:12:ARG:HH11  | 32:B7:12:ARG:HG3   | 1.79                     | 0.46              |
| 33:B8:4:MET:O      | 33:B8:62:LEU:CD1   | 2.60                     | 0.46              |
| 35:BA:1045:A:O2'   | 35:BA:1047:G:C5    | 2.68                     | 0.46              |
| 27:B2:69:ARG:HH12  | 35:BA:111:A:H5'    | 1.79                     | 0.46              |
| 35:BA:1555:G:H2'   | 35:BA:1555:G:N3    | 2.30                     | 0.46              |
| 35:BA:1680:U:H2'   | 35:BA:1681:G:O4'   | 2.14                     | 0.46              |
| 35:BA:2305:A:H2'   | 35:BA:2306:C:O4'   | 2.15                     | 0.46              |
| 35:BA:2476:A:C2    | 35:BA:2477:C:C6    | 3.03                     | 0.46              |
| 35:BA:271(J):C:C2' | 35:BA:271(J):C:O2  | 2.63                     | 0.46              |
| 35:BA:2820:A:HO2'  | 35:BA:2821:A:P     | 2.36                     | 0.46              |
| 35:BA:718:A:H2'    | 35:BA:719:C:O4'    | 2.16                     | 0.46              |
| 37:BC:79:ALA:O     | 37:BC:120:VAL:HG11 | 2.15                     | 0.46              |
| 38:BD:77:ALA:HB2   | 38:BD:97:TYR:HA    | 1.97                     | 0.46              |
| 35:BA:2579:C:O3'   | 39:BE:131:ALA:HB2  | 2.15                     | 0.46              |
| 39:BE:68:ALA:HB3   | 39:BE:69:LYS:HE2   | 1.98                     | 0.46              |
| 40:BF:3:GLU:CB     | 40:BF:24:LEU:HG    | 2.43                     | 0.46              |
| 40:BF:2:LYS:CG     | 40:BF:25:PRO:HG2   | 2.45                     | 0.46              |
| 41:BG:9:ARG:HD3    | 41:BG:13:GLU:OE1   | 2.15                     | 0.46              |
| 29:B4:1:MET:CE     | 41:BG:66:GLN:OE1   | 2.63                     | 0.46              |
| 42:BH:41:MET:HE2   | 42:BH:42:ARG:C     | 2.36                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 44:BK:93:ARG:HD2   | 44:BK:93:ARG:C      | 2.35                     | 0.46              |
| 46:BN:15:LEU:O     | 46:BN:136:GLU:HA    | 2.16                     | 0.46              |
| 48:BP:106:LEU:HD11 | 48:BP:112:LEU:HD23  | 1.97                     | 0.46              |
| 49:BQ:12:GLN:HE21  | 49:BQ:73:PRO:CD     | 2.27                     | 0.46              |
| 50:BR:44:LEU:HD13  | 50:BR:44:LEU:C      | 2.35                     | 0.46              |
| 50:BR:51:LEU:HD12  | 50:BR:51:LEU:H      | 1.80                     | 0.46              |
| 53:BU:66:ASN:O     | 53:BU:68:ALA:N      | 2.48                     | 0.46              |
| 57:BY:37:VAL:HG23  | 57:BY:38:ILE:N      | 2.30                     | 0.46              |
| 58:BZ:144:LEU:HD11 | 58:BZ:150:LEU:HD22  | 1.96                     | 0.46              |
| 1:CA:1512:U:H2'    | 1:CA:1513:A:H8      | 1.80                     | 0.46              |
| 1:CA:308:C:H2'     | 1:CA:309:G:H8       | 1.80                     | 0.46              |
| 1:CA:965:A:C2      | 1:CA:969:A:N1       | 2.83                     | 0.46              |
| 3:CC:115:LEU:O     | 3:CC:116:VAL:C      | 2.54                     | 0.46              |
| 3:CC:136:GLN:O     | 3:CC:137:ALA:C      | 2.52                     | 0.46              |
| 4:CD:165:MET:HE2   | 4:CD:176:LEU:CD2    | 2.46                     | 0.46              |
| 4:CD:29:PRO:O      | 4:CD:30:LYS:CB      | 2.61                     | 0.46              |
| 5:CE:8:GLU:HA      | 5:CE:34:VAL:HA      | 1.96                     | 0.46              |
| 10:CJ:61:GLU:HG3   | 14:CN:58:LYS:HZ3    | 1.80                     | 0.46              |
| 10:CJ:79:ARG:HH11  | 10:CJ:79:ARG:N      | 2.13                     | 0.46              |
| 12:CL:110:VAL:CG2  | 12:CL:120:TYR:HB3   | 2.44                     | 0.46              |
| 12:CL:24:VAL:O     | 12:CL:24:VAL:HG12   | 2.16                     | 0.46              |
| 13:CM:22:ILE:HD12  | 13:CM:22:ILE:N      | 2.29                     | 0.46              |
| 16:CP:20:VAL:HG23  | 16:CP:34:GLU:O      | 2.15                     | 0.46              |
| 16:CP:2:VAL:O      | 16:CP:2:VAL:HG22    | 2.14                     | 0.46              |
| 17:CQ:45:HIS:CG    | 17:CQ:65:ILE:HD13   | 2.50                     | 0.46              |
| 18:CR:40:LEU:C     | 18:CR:42:ARG:H      | 2.19                     | 0.46              |
| 19:CS:11:VAL:HG13  | 19:CS:11:VAL:O      | 2.16                     | 0.46              |
| 20:CT:86:ARG:NH1   | 20:CT:86:ARG:HG3    | 2.30                     | 0.46              |
| 22:CW:8:U:H3       | 22:CW:14:A:H62      | 1.62                     | 0.46              |
| 24:CY:216:LEU:O    | 24:CY:220:ALA:N     | 2.46                     | 0.46              |
| 24:CY:319:ASP:OD2  | 24:CY:322:VAL:HG22  | 2.15                     | 0.46              |
| 24:CY:34:TYR:O     | 24:CY:38:ARG:HB2    | 2.15                     | 0.46              |
| 24:CY:530:VAL:HG13 | 24:CY:531:GLY:N     | 2.29                     | 0.46              |
| 25:D0:51:VAL:HG22  | 25:D0:81:VAL:CG2    | 2.43                     | 0.46              |
| 26:D1:81:LYS:HZ3   | 35:DA:271(H):G:H5'' | 1.79                     | 0.46              |
| 27:D2:69:ARG:HH22  | 35:DA:111:A:C4'     | 2.28                     | 0.46              |
| 29:D4:14:ILE:HD13  | 29:D4:22:ILE:C      | 2.36                     | 0.46              |
| 30:D5:36:CYS:SG    | 30:D5:49:CYS:HB3    | 2.55                     | 0.46              |
| 31:D6:43:CYS:CB    | 31:D6:44:ARG:HH21   | 2.23                     | 0.46              |
| 31:D6:9:LEU:HD13   | 31:D6:9:LEU:O       | 2.15                     | 0.46              |
| 33:D8:48:PHE:HB3   | 33:D8:49:VAL:H      | 1.45                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:DA:1181:C:O2'  | 35:DA:1182:A:H5'   | 2.15                     | 0.46              |
| 35:DA:1326:U:H5'' | 35:DA:2011:U:H1'   | 1.96                     | 0.46              |
| 35:DA:1362:C:H2'  | 35:DA:1363:C:H6    | 1.80                     | 0.46              |
| 35:DA:1448:G:N3   | 35:DA:1528(A):A:H2 | 2.13                     | 0.46              |
| 35:DA:1843:C:H2'  | 35:DA:1844:C:H6    | 1.78                     | 0.46              |
| 35:DA:2137:C:O2'  | 35:DA:2138:C:H5'   | 2.15                     | 0.46              |
| 35:DA:2001:A:H4'  | 35:DA:2689:U:H2'   | 1.98                     | 0.46              |
| 35:DA:345:A:O2'   | 35:DA:346:A:N7     | 2.47                     | 0.46              |
| 35:DA:604:G:O2'   | 35:DA:605:C:H5'    | 2.15                     | 0.46              |
| 35:DA:725:G:C6    | 35:DA:726:G:N1     | 2.83                     | 0.46              |
| 35:DA:733:G:O6    | 35:DA:761:A:C8     | 2.68                     | 0.46              |
| 35:DA:797:C:P     | 40:DF:62:ARG:HG3   | 2.55                     | 0.46              |
| 35:DA:894:C:C2'   | 35:DA:895:U:H5'    | 2.46                     | 0.46              |
| 39:DE:68:ALA:O    | 39:DE:70:ALA:N     | 2.48                     | 0.46              |
| 40:DF:18:ARG:CZ   | 40:DF:199:TRP:CZ3  | 2.98                     | 0.46              |
| 46:DN:87:LEU:O    | 46:DN:88:GLU:C     | 2.53                     | 0.46              |
| 46:DN:90:MET:HB3  | 46:DN:98:VAL:HG22  | 1.97                     | 0.46              |
| 47:DO:114:ILE:H   | 47:DO:114:ILE:CD1  | 2.22                     | 0.46              |
| 35:DA:2393:A:H5'  | 48:DP:60:MET:O     | 2.15                     | 0.46              |
| 49:DQ:21:THR:CG2  | 49:DQ:101:ARG:HB2  | 2.44                     | 0.46              |
| 51:DS:42:ASP:O    | 51:DS:43:GLU:HB2   | 2.15                     | 0.46              |
| 52:DT:102:ILE:HB  | 52:DT:110:ILE:CD1  | 2.45                     | 0.46              |
| 52:DT:118:ARG:HA  | 52:DT:121:ILE:CB   | 2.40                     | 0.46              |
| 53:DU:83:LEU:CD1  | 53:DU:83:LEU:N     | 2.73                     | 0.46              |
| 55:DW:25:ARG:HB2  | 55:DW:25:ARG:NH1   | 2.30                     | 0.46              |
| 57:DY:68:HIS:CB   | 57:DY:71:LYS:HZ3   | 2.28                     | 0.46              |
| 58:DZ:61:LEU:N    | 58:DZ:65:GLN:O     | 2.43                     | 0.46              |
| 1:AA:719:C:O2     | 18:AR:50:ILE:HG12  | 2.15                     | 0.46              |
| 2:AB:189:ASP:OD2  | 2:AB:205:ASP:OD1   | 2.33                     | 0.46              |
| 2:AB:229:VAL:HG12 | 2:AB:230:VAL:N     | 2.31                     | 0.46              |
| 2:AB:233:SER:CB   | 2:AB:234:PRO:HD2   | 2.44                     | 0.46              |
| 3:AC:136:GLN:O    | 3:AC:137:ALA:C     | 2.52                     | 0.46              |
| 3:AC:32:LEU:HB3   | 3:AC:59:ARG:HH22   | 1.81                     | 0.46              |
| 4:AD:101:LEU:HD23 | 4:AD:121:VAL:CG1   | 2.45                     | 0.46              |
| 5:AE:11:ILE:HD13  | 5:AE:105:VAL:HG13  | 1.97                     | 0.46              |
| 5:AE:78:HIS:CE1   | 5:AE:80:ILE:HG23   | 2.50                     | 0.46              |
| 7:AG:18:TYR:HD2   | 7:AG:59:LEU:HD13   | 1.79                     | 0.46              |
| 10:AJ:63:PHE:HB2  | 14:AN:57:ARG:O     | 2.15                     | 0.46              |
| 12:AL:58:VAL:O    | 12:AL:65:GLU:HA    | 2.14                     | 0.46              |
| 1:AA:190:U:O2     | 20:AT:105:SER:HB2  | 2.15                     | 0.46              |
| 24:AY:122:TRP:CD1 | 24:AY:122:TRP:C    | 2.88                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:AY:227:ILE:CD1  | 24:AY:242:LEU:HA   | 2.45                     | 0.46              |
| 24:AY:337:SER:HB2  | 24:AY:355:LEU:HD23 | 1.98                     | 0.46              |
| 24:AY:625:ASN:C    | 24:AY:627:ARG:H    | 2.18                     | 0.46              |
| 24:AY:605:ILE:HD11 | 24:AY:677:GLN:HG2  | 1.97                     | 0.46              |
| 26:B1:94:LEU:O     | 26:B1:96:LYS:N     | 2.48                     | 0.46              |
| 27:B2:24:LEU:O     | 27:B2:27:GLU:HB2   | 2.15                     | 0.46              |
| 27:B2:37:PHE:O     | 27:B2:41:ILE:HG23  | 2.14                     | 0.46              |
| 28:B3:19:GLN:O     | 28:B3:22:ALA:HB3   | 2.16                     | 0.46              |
| 30:B5:16:ARG:NH2   | 35:BA:517:C:OP1    | 2.48                     | 0.46              |
| 31:B6:8:LYS:CE     | 31:B6:25:LYS:HD3   | 2.35                     | 0.46              |
| 31:B6:5:VAL:HG22   | 35:BA:2283:C:OP1   | 2.15                     | 0.46              |
| 35:BA:1161:C:H2'   | 35:BA:1162:G:H8    | 1.80                     | 0.46              |
| 35:BA:134:C:O2'    | 35:BA:135:G:H5'    | 2.15                     | 0.46              |
| 35:BA:205:G:O2'    | 35:BA:206:U:OP2    | 2.31                     | 0.46              |
| 35:BA:2190:G:O2'   | 35:BA:2191:G:H5'   | 2.16                     | 0.46              |
| 35:BA:2795:G:H2'   | 35:BA:2795:G:N3    | 2.30                     | 0.46              |
| 35:BA:2845:G:O5'   | 35:BA:2845:G:H8    | 1.97                     | 0.46              |
| 35:BA:996:A:H2'    | 35:BA:997:G:H8     | 1.80                     | 0.46              |
| 36:BB:66:A:N6      | 36:BB:108:U:H2'    | 2.23                     | 0.46              |
| 37:BC:185:LYS:HE3  | 37:BC:185:LYS:CA   | 2.45                     | 0.46              |
| 37:BC:86:GLU:O     | 37:BC:90:ALA:HB2   | 2.16                     | 0.46              |
| 41:BG:98:ARG:O     | 41:BG:102:PHE:HB2  | 2.14                     | 0.46              |
| 41:BG:164:GLU:O    | 41:BG:165:THR:HG23 | 2.15                     | 0.46              |
| 41:BG:172:LEU:HD23 | 41:BG:172:LEU:C    | 2.35                     | 0.46              |
| 41:BG:61:ALA:O     | 41:BG:65:GLY:N     | 2.48                     | 0.46              |
| 44:BK:99:ILE:O     | 44:BK:139:VAL:N    | 2.47                     | 0.46              |
| 46:BN:134:ARG:O    | 46:BN:134:ARG:HG3  | 2.16                     | 0.46              |
| 46:BN:26:LEU:HD12  | 46:BN:26:LEU:O     | 2.15                     | 0.46              |
| 46:BN:57:ALA:O     | 46:BN:58:ASP:O     | 2.32                     | 0.46              |
| 48:BP:122:PRO:HA   | 48:BP:141:ALA:O    | 2.16                     | 0.46              |
| 49:BQ:56:ARG:CA    | 49:BQ:56:ARG:NE    | 2.75                     | 0.46              |
| 50:BR:101:ALA:O    | 50:BR:102:GLU:HB2  | 2.14                     | 0.46              |
| 51:BS:104:GLY:C    | 51:BS:106:ARG:N    | 2.67                     | 0.46              |
| 53:BU:21:ALA:HA    | 53:BU:24:TYR:CD1   | 2.50                     | 0.46              |
| 53:BU:90:VAL:O     | 53:BU:91:ASP:C     | 2.53                     | 0.46              |
| 54:BV:38:LEU:C     | 54:BV:39:LEU:HD13  | 2.34                     | 0.46              |
| 57:BY:52:SER:N     | 57:BY:53:PRO:HD2   | 2.30                     | 0.46              |
| 57:BY:84:ARG:HD2   | 57:BY:97:ARG:HD2   | 1.97                     | 0.46              |
| 58:BZ:127:LYS:O    | 58:BZ:128:VAL:HB   | 2.16                     | 0.46              |
| 58:BZ:24:LEU:HD21  | 58:BZ:86:VAL:HG23  | 1.96                     | 0.46              |
| 1:CA:1030:C:N4     | 1:CA:1032:G:C2     | 2.83                     | 0.46              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1351:U:O2'    | 1:CA:1352:C:H5'    | 2.15                     | 0.46              |
| 1:CA:620:C:H2'     | 1:CA:621:A:C8      | 2.50                     | 0.46              |
| 2:CB:51:LEU:O      | 2:CB:55:PHE:HD2    | 1.96                     | 0.46              |
| 3:CC:82:GLU:N      | 3:CC:82:GLU:OE2    | 2.49                     | 0.46              |
| 5:CE:143:ARG:HA    | 5:CE:143:ARG:HD3   | 1.72                     | 0.46              |
| 10:CJ:5:ARG:HA     | 10:CJ:73:ASP:OD1   | 2.15                     | 0.46              |
| 12:CL:42:THR:HG23  | 12:CL:42:THR:O     | 2.14                     | 0.46              |
| 12:CL:92:ASP:O     | 12:CL:94:PRO:HD3   | 2.14                     | 0.46              |
| 13:CM:86:CYS:HA    | 19:CS:73:GLU:O     | 2.15                     | 0.46              |
| 16:CP:14:ASN:N     | 16:CP:15:PRO:CD    | 2.78                     | 0.46              |
| 16:CP:27:LYS:HG2   | 16:CP:30:GLY:HA3   | 1.97                     | 0.46              |
| 19:CS:19:VAL:HG13  | 19:CS:44:MET:HG2   | 1.96                     | 0.46              |
| 20:CT:30:LYS:HZ2   | 20:CT:34:LYS:CE    | 2.29                     | 0.46              |
| 21:CU:2:GLY:C      | 21:CU:4:GLY:N      | 2.69                     | 0.46              |
| 24:CY:255:ILE:CG1  | 24:CY:256:THR:N    | 2.78                     | 0.46              |
| 24:CY:314:PHE:O    | 24:CY:315:LYS:HB2  | 2.15                     | 0.46              |
| 27:D2:4:SER:O      | 27:D2:5:GLU:C      | 2.54                     | 0.46              |
| 33:D8:50:LEU:C     | 33:D8:53:PRO:CD    | 2.83                     | 0.46              |
| 35:DA:1097:U:C2'   | 35:DA:1098:A:H5'   | 2.45                     | 0.46              |
| 35:DA:1237:A:O2'   | 35:DA:1238:G:P     | 2.73                     | 0.46              |
| 35:DA:1263:U:C4    | 35:DA:1264:G:C6    | 3.03                     | 0.46              |
| 35:DA:1472:A:O2'   | 35:DA:1473:G:H5'   | 2.15                     | 0.46              |
| 35:DA:1484:G:H2'   | 35:DA:1485:G:H5''  | 1.97                     | 0.46              |
| 35:DA:1630:G:C2    | 35:DA:1637:A:C2    | 3.03                     | 0.46              |
| 35:DA:1770:G:C2'   | 35:DA:1771:C:H5'   | 2.45                     | 0.46              |
| 35:DA:1783:A:C2    | 35:DA:2587:A:C4    | 3.04                     | 0.46              |
| 35:DA:2012:G:H4'   | 55:DW:96:ILE:CD1   | 2.19                     | 0.46              |
| 35:DA:2389:G:C5'   | 35:DA:2390:U:H5'   | 2.39                     | 0.46              |
| 35:DA:2521:C:H2'   | 35:DA:2521:C:O2    | 2.14                     | 0.46              |
| 35:DA:2712:U:O2'   | 35:DA:2712(A):A:C8 | 2.43                     | 0.46              |
| 35:DA:247:G:H4'    | 35:DA:386:G:C5     | 2.49                     | 0.46              |
| 35:DA:833:U:O2     | 48:DP:55:ARG:NH1   | 2.47                     | 0.46              |
| 35:DA:958:U:C6     | 35:DA:958:U:C3'    | 2.99                     | 0.46              |
| 38:DD:26:LYS:O     | 38:DD:27:THR:HB    | 2.15                     | 0.46              |
| 35:DA:1353:A:H4'   | 38:DD:38:LYS:HE3   | 1.96                     | 0.46              |
| 38:DD:53:PHE:HA    | 38:DD:218:ARG:HB2  | 1.98                     | 0.46              |
| 38:DD:9:TYR:CD2    | 38:DD:10:THR:HG22  | 2.49                     | 0.46              |
| 40:DF:160:ASN:HD21 | 40:DF:162:LEU:CD1  | 2.28                     | 0.46              |
| 40:DF:38:ARG:O     | 40:DF:42:ALA:CB    | 2.62                     | 0.46              |
| 40:DF:4:VAL:HA     | 40:DF:19:GLU:HB3   | 1.96                     | 0.46              |
| 41:DG:131:TYR:HE2  | 41:DG:133:LEU:CD2  | 2.25                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:2312:U:H2'   | 41:DG:40:ASN:OD1   | 2.16                     | 0.46              |
| 41:DG:7:LEU:O      | 41:DG:8:LYS:C      | 2.53                     | 0.46              |
| 42:DH:33:LEU:HD21  | 42:DH:136:ILE:HG22 | 1.96                     | 0.46              |
| 44:DK:108:ALA:O    | 44:DK:112:MET:HB3  | 2.15                     | 0.46              |
| 35:DA:1081:U:H4'   | 44:DK:117:THR:HG21 | 1.96                     | 0.46              |
| 46:DN:65:LYS:NZ    | 46:DN:65:LYS:CB    | 2.78                     | 0.46              |
| 48:DP:29:LYS:HB3   | 48:DP:34:GLY:H     | 1.80                     | 0.46              |
| 35:DA:1275:A:C4    | 50:DR:16:HIS:ND1   | 2.83                     | 0.46              |
| 51:DS:11:LYS:N     | 51:DS:11:LYS:HD2   | 2.29                     | 0.46              |
| 51:DS:47:THR:CG2   | 51:DS:49:VAL:O     | 2.63                     | 0.46              |
| 51:DS:89:ARG:NH1   | 51:DS:89:ARG:HG2   | 2.28                     | 0.46              |
| 1:AA:108:G:N2      | 1:AA:109:A:C2      | 2.83                     | 0.46              |
| 1:AA:1164:G:O2'    | 1:AA:1165:C:H5'    | 2.15                     | 0.46              |
| 1:AA:1226:C:C5     | 13:AM:104:ARG:HB2  | 2.50                     | 0.46              |
| 1:AA:182:U:H5'     | 1:AA:183:G:P       | 2.55                     | 0.46              |
| 1:AA:203:U:H5'     | 1:AA:216:G:N2      | 2.30                     | 0.46              |
| 1:AA:265:G:H5'     | 17:AQ:64:PRO:O     | 2.15                     | 0.46              |
| 1:AA:276:G:O2'     | 1:AA:277:C:H5'     | 2.15                     | 0.46              |
| 1:AA:773:G:C2'     | 1:AA:774:G:H5'     | 2.46                     | 0.46              |
| 2:AB:15:VAL:C      | 2:AB:16:HIS:CG     | 2.88                     | 0.46              |
| 2:AB:88:ALA:HB2    | 2:AB:219:VAL:CG1   | 2.44                     | 0.46              |
| 3:AC:138:VAL:O     | 3:AC:140:ARG:N     | 2.49                     | 0.46              |
| 3:AC:80:GLY:HA3    | 3:AC:82:GLU:OE1    | 2.15                     | 0.46              |
| 5:AE:101:ILE:HD11  | 5:AE:119:LEU:CD2   | 2.46                     | 0.46              |
| 5:AE:76:ILE:CG1    | 5:AE:77:PRO:HD2    | 2.45                     | 0.46              |
| 13:AM:99:ARG:O     | 13:AM:100:GLY:C    | 2.53                     | 0.46              |
| 16:AP:67:THR:HG22  | 16:AP:68:ASP:H     | 1.80                     | 0.46              |
| 24:AY:277:VAL:HG13 | 24:AY:278:ASP:N    | 2.31                     | 0.46              |
| 26:B1:44:PRO:HG2   | 26:B1:46:LEU:HD11  | 1.97                     | 0.46              |
| 29:B4:9:LEU:HD13   | 29:B4:10:VAL:H     | 1.79                     | 0.46              |
| 29:B4:9:LEU:HD12   | 29:B4:10:VAL:H     | 1.81                     | 0.46              |
| 30:B5:36:CYS:SG    | 30:B5:49:CYS:HB3   | 2.54                     | 0.46              |
| 35:BA:1516:C:H2'   | 35:BA:1517:G:H5''  | 1.95                     | 0.46              |
| 35:BA:1721:G:O6    | 35:BA:1739:U:H5'   | 2.15                     | 0.46              |
| 35:BA:1812:A:H2'   | 35:BA:1813:G:C8    | 2.45                     | 0.46              |
| 35:BA:2291:U:OP1   | 35:BA:2380:C:O2'   | 2.33                     | 0.46              |
| 35:BA:2291:U:O2'   | 35:BA:2292:C:H5'   | 2.14                     | 0.46              |
| 35:BA:360:G:H2'    | 35:BA:361:G:H8     | 1.80                     | 0.46              |
| 35:BA:578:A:H5'    | 35:BA:1254:A:OP1   | 2.16                     | 0.46              |
| 35:BA:602:G:C2     | 35:BA:656:G:C6     | 3.03                     | 0.46              |
| 35:BA:754:C:H2'    | 35:BA:755:C:C6     | 2.50                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:975:C:OP2    | 35:BA:975:C:H4'    | 2.16                     | 0.46              |
| 38:BD:148:GLU:HB2  | 38:BD:151:LYS:CG   | 2.45                     | 0.46              |
| 38:BD:92:ILE:HD13  | 38:BD:92:ILE:H     | 1.79                     | 0.46              |
| 41:BG:173:LEU:O    | 41:BG:178:PHE:HD1  | 1.99                     | 0.46              |
| 41:BG:181:ARG:O    | 41:BG:182:LYS:C    | 2.54                     | 0.46              |
| 42:BH:65:HIS:HE1   | 42:BH:69:ARG:NH1   | 2.14                     | 0.46              |
| 44:BK:37:PHE:C     | 44:BK:39:LYS:H     | 2.17                     | 0.46              |
| 46:BN:15:LEU:CD2   | 46:BN:53:VAL:HB    | 2.45                     | 0.46              |
| 46:BN:61:ARG:HG3   | 46:BN:61:ARG:HH11  | 1.81                     | 0.46              |
| 48:BP:100:LEU:HD22 | 48:BP:100:LEU:N    | 2.30                     | 0.46              |
| 49:BQ:55:VAL:HG12  | 49:BQ:56:ARG:H     | 1.80                     | 0.46              |
| 50:BR:9:LYS:O      | 50:BR:10:LEU:CD2   | 2.60                     | 0.46              |
| 51:BS:35:ILE:HD11  | 51:BS:99:LYS:HE3   | 1.97                     | 0.46              |
| 52:BT:137:LYS:HG2  | 52:BT:138:ALA:N    | 2.30                     | 0.46              |
| 52:BT:50:ILE:HG23  | 52:BT:99:LEU:O     | 2.16                     | 0.46              |
| 53:BU:53:ARG:O     | 53:BU:56:ASP:N     | 2.37                     | 0.46              |
| 53:BU:53:ARG:CA    | 53:BU:56:ASP:OD2   | 2.60                     | 0.46              |
| 35:BA:487:C:H1'    | 55:BW:53:SER:HA    | 1.95                     | 0.46              |
| 35:BA:747:U:O2'    | 55:BW:88:ARG:HG3   | 2.16                     | 0.46              |
| 57:BY:42:VAL:O     | 57:BY:65:ALA:N     | 2.39                     | 0.46              |
| 58:BZ:41:LEU:O     | 58:BZ:42:VAL:C     | 2.53                     | 0.46              |
| 1:CA:1010:G:C6     | 1:CA:1020:U:H1'    | 2.50                     | 0.46              |
| 1:CA:357:G:O2'     | 1:CA:358:U:H5'     | 2.15                     | 0.46              |
| 1:CA:794:A:O2'     | 1:CA:795:C:H5'     | 2.15                     | 0.46              |
| 1:CA:973:G:C1'     | 10:CJ:55:LYS:HE2   | 2.44                     | 0.46              |
| 1:CA:98:G:H2'      | 1:CA:99:U:O4'      | 2.15                     | 0.46              |
| 2:CB:204:ASN:C     | 2:CB:204:ASN:ND2   | 2.62                     | 0.46              |
| 2:CB:222:ILE:HB    | 2:CB:226:ARG:NH2   | 2.28                     | 0.46              |
| 3:CC:187:ALA:C     | 3:CC:188:LEU:HD22  | 2.36                     | 0.46              |
| 3:CC:206:GLU:HG2   | 3:CC:207:VAL:N     | 2.28                     | 0.46              |
| 4:CD:13:ARG:O      | 4:CD:14:ARG:C      | 2.54                     | 0.46              |
| 4:CD:191:ARG:NH1   | 4:CD:191:ARG:O     | 2.49                     | 0.46              |
| 5:CE:101:ILE:HD11  | 5:CE:119:LEU:CD2   | 2.45                     | 0.46              |
| 7:CG:44:TYR:HA     | 7:CG:47:CYS:SG     | 2.55                     | 0.46              |
| 8:CH:32:LYS:C      | 8:CH:34:GLU:N      | 2.68                     | 0.46              |
| 9:CI:56:LEU:C      | 9:CI:56:LEU:HD23   | 2.35                     | 0.46              |
| 1:CA:322:C:H4'     | 20:CT:23:ARG:HD2   | 1.97                     | 0.46              |
| 24:CY:18:ALA:O     | 24:CY:106:VAL:HA   | 2.15                     | 0.46              |
| 24:CY:527:ASN:HD22 | 24:CY:527:ASN:C    | 2.18                     | 0.46              |
| 24:CY:631:ILE:O    | 24:CY:632:LEU:HD23 | 2.15                     | 0.46              |
| 31:D6:27:LYS:CD    | 31:D6:30:THR:HB    | 2.44                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:D6:43:CYS:O     | 31:D6:44:ARG:NE    | 2.48                     | 0.46              |
| 31:D6:54:ILE:O     | 31:D6:54:ILE:CG1   | 2.63                     | 0.46              |
| 32:D7:12:ARG:HG3   | 32:D7:12:ARG:HH11  | 1.80                     | 0.46              |
| 34:D9:17:ILE:HG22  | 34:D9:18:ARG:H     | 1.80                     | 0.46              |
| 35:DA:1718:G:C5'   | 35:DA:1718:G:H8    | 2.26                     | 0.46              |
| 35:DA:176:G:C2'    | 35:DA:177:G:H5'    | 2.44                     | 0.46              |
| 35:DA:2291:U:O2'   | 35:DA:2292:C:H5'   | 2.14                     | 0.46              |
| 35:DA:2464:C:O2'   | 35:DA:2465:C:O5'   | 2.33                     | 0.46              |
| 35:DA:2787:C:H2'   | 35:DA:2787:C:O2    | 2.15                     | 0.46              |
| 35:DA:484:C:O2'    | 35:DA:485:C:H5'    | 2.15                     | 0.46              |
| 35:DA:614:U:H2'    | 35:DA:614(A):U:O4' | 2.15                     | 0.46              |
| 35:DA:665:C:O2'    | 35:DA:666:G:H5'    | 2.15                     | 0.46              |
| 36:DB:82:G:HO2'    | 36:DB:83:G:H5'     | 1.81                     | 0.46              |
| 37:DC:60:ARG:HG3   | 37:DC:165:ARG:HG3  | 1.97                     | 0.46              |
| 37:DC:46:ALA:HA    | 37:DC:212:SER:O    | 2.15                     | 0.46              |
| 38:DD:138:VAL:HA   | 38:DD:165:ILE:HG21 | 1.98                     | 0.46              |
| 38:DD:197:GLY:O    | 38:DD:198:ASN:HB3  | 2.16                     | 0.46              |
| 38:DD:218:ARG:HB3  | 38:DD:219:PRO:HD2  | 1.96                     | 0.46              |
| 40:DF:132:VAL:CG2  | 40:DF:133:ASN:N    | 2.78                     | 0.46              |
| 40:DF:26:ALA:O     | 40:DF:27:GLU:HG3   | 2.15                     | 0.46              |
| 41:DG:34:LEU:CD1   | 41:DG:34:LEU:H     | 2.17                     | 0.46              |
| 41:DG:72:ARG:HB3   | 41:DG:87:PRO:HD2   | 1.96                     | 0.46              |
| 42:DH:65:HIS:HE1   | 42:DH:69:ARG:NH1   | 2.10                     | 0.46              |
| 24:CY:636:PRO:HG3  | 44:DK:20:ALA:HB1   | 1.97                     | 0.46              |
| 46:DN:57:ALA:O     | 46:DN:58:ASP:O     | 2.33                     | 0.46              |
| 47:DO:64:ARG:NH1   | 47:DO:83:ALA:HB2   | 2.30                     | 0.46              |
| 48:DP:106:LEU:HD21 | 48:DP:112:LEU:HG   | 1.97                     | 0.46              |
| 50:DR:97:VAL:HG13  | 50:DR:114:VAL:CG2  | 2.46                     | 0.46              |
| 52:DT:10:VAL:O     | 52:DT:11:GLU:C     | 2.53                     | 0.46              |
| 52:DT:53:ARG:O     | 52:DT:59:THR:HB    | 2.15                     | 0.46              |
| 57:DY:56:PRO:O     | 57:DY:57:GLN:HB3   | 2.16                     | 0.46              |
| 35:DA:336:C:H4'    | 57:DY:7:VAL:CG2    | 2.45                     | 0.46              |
| 58:DZ:92:SER:HB3   | 58:DZ:93:ASP:H     | 1.47                     | 0.46              |
| 1:AA:1053:G:N7     | 1:AA:1200:C:C5'    | 2.73                     | 0.46              |
| 1:AA:1217:C:H2'    | 1:AA:1217:C:O2     | 2.15                     | 0.46              |
| 1:AA:1392:G:O2'    | 1:AA:1393:U:H5'    | 2.16                     | 0.46              |
| 1:AA:720:C:C3'     | 1:AA:721:G:H5''    | 2.35                     | 0.46              |
| 1:AA:759:A:C2'     | 1:AA:760:G:H5'     | 2.45                     | 0.46              |
| 3:AC:3:ASN:N       | 3:AC:3:ASN:OD1     | 2.48                     | 0.46              |
| 4:AD:173:TRP:O     | 4:AD:174:LEU:HD23  | 2.16                     | 0.46              |
| 4:AD:194:LEU:HB3   | 4:AD:196:LEU:CD1   | 2.36                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 4:AD:57:ARG:NH1    | 4:AD:205:GLU:OE2    | 2.48                     | 0.46              |
| 5:AE:155:GLU:N     | 8:AH:64:LYS:HE2     | 2.31                     | 0.46              |
| 5:AE:28:PHE:O      | 5:AE:47:LYS:HA      | 2.15                     | 0.46              |
| 7:AG:97:GLN:O      | 7:AG:98:SER:C       | 2.53                     | 0.46              |
| 8:AH:32:LYS:C      | 8:AH:34:GLU:N       | 2.65                     | 0.46              |
| 12:AL:28:LYS:HB2   | 12:AL:33:ARG:HH22   | 1.81                     | 0.46              |
| 24:AY:100:VAL:HG13 | 24:AY:101:LEU:H     | 1.81                     | 0.46              |
| 24:AY:379:GLY:O    | 24:AY:380:LEU:O     | 2.33                     | 0.46              |
| 24:AY:71:THR:HA    | 24:AY:79:ILE:O      | 2.16                     | 0.46              |
| 25:B0:20:ARG:CG    | 25:B0:20:ARG:HH11   | 2.29                     | 0.46              |
| 29:B4:2:LYS:HB2    | 36:BB:40:U:O4       | 2.16                     | 0.46              |
| 35:BA:1448:G:N3    | 35:BA:1528(A):A:H2  | 2.13                     | 0.46              |
| 35:BA:1485:G:H1'   | 35:BA:1505:C:N4     | 2.23                     | 0.46              |
| 35:BA:1528:A:O2'   | 35:BA:1528(A):A:O5' | 2.32                     | 0.46              |
| 35:BA:1851:U:H2'   | 35:BA:1852:C:O4'    | 2.16                     | 0.46              |
| 35:BA:1952:A:C2    | 47:BO:22:ILE:HG23   | 2.50                     | 0.46              |
| 35:BA:827:U:H2'    | 35:BA:2068:U:O2     | 2.15                     | 0.46              |
| 35:BA:2081:C:H2'   | 35:BA:2082:A:H8     | 1.79                     | 0.46              |
| 35:BA:2523:G:C3'   | 35:BA:2524:G:H5''   | 2.45                     | 0.46              |
| 35:BA:272(G):C:C3' | 35:BA:272(H):C:H5'' | 2.45                     | 0.46              |
| 35:BA:729:G:O2'    | 35:BA:763:G:H4'     | 2.15                     | 0.46              |
| 35:BA:79:G:O2'     | 35:BA:80:G:H5'      | 2.15                     | 0.46              |
| 35:BA:94(A):G:H2'  | 35:BA:95:G:H5''     | 1.96                     | 0.46              |
| 38:BD:127:VAL:HA   | 38:BD:193:VAL:HG13  | 1.96                     | 0.46              |
| 39:BE:24:THR:CG2   | 39:BE:184:VAL:HG23  | 2.37                     | 0.46              |
| 40:BF:101:LEU:O    | 40:BF:106:ARG:NH1   | 2.49                     | 0.46              |
| 42:BH:138:LYS:C    | 42:BH:140:LYS:N     | 2.69                     | 0.46              |
| 44:BK:100:THR:CA   | 44:BK:139:VAL:HB    | 2.41                     | 0.46              |
| 46:BN:133:GLN:HG2  | 46:BN:134:ARG:H     | 1.81                     | 0.46              |
| 46:BN:90:MET:HB3   | 46:BN:98:VAL:HG22   | 1.97                     | 0.46              |
| 48:BP:106:LEU:HD21 | 48:BP:112:LEU:HG    | 1.97                     | 0.46              |
| 35:BA:2406:U:N3    | 48:BP:72:PRO:HB2    | 2.30                     | 0.46              |
| 49:BQ:43:THR:HB    | 49:BQ:45:GLN:HE21   | 1.80                     | 0.46              |
| 49:BQ:79:LEU:HD23  | 49:BQ:80:GLU:N      | 2.28                     | 0.46              |
| 50:BR:7:GLY:C      | 50:BR:8:ARG:HE      | 2.19                     | 0.46              |
| 52:BT:29:ARG:HG3   | 52:BT:30:VAL:HG13   | 1.97                     | 0.46              |
| 52:BT:29:ARG:HG2   | 52:BT:85:LYS:HA     | 1.96                     | 0.46              |
| 53:BU:55:ARG:HA    | 53:BU:58:ARG:HB2    | 1.98                     | 0.46              |
| 53:BU:82:GLY:O     | 53:BU:84:LYS:N      | 2.48                     | 0.46              |
| 53:BU:98:LEU:O     | 53:BU:106:PHE:HB2   | 2.16                     | 0.46              |
| 54:BV:31:ALA:C     | 54:BV:61:VAL:HG12   | 2.36                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:BX:43:VAL:C     | 56:BX:45:THR:H     | 2.18                     | 0.46              |
| 1:CA:1003:G:H1'    | 1:CA:1039:C:O2     | 2.15                     | 0.46              |
| 1:CA:1237:C:H3'    | 1:CA:1336:C:N4     | 2.31                     | 0.46              |
| 1:CA:17:U:H2'      | 1:CA:18:C:C6       | 2.50                     | 0.46              |
| 1:CA:192:U:C4'     | 20:CT:103:GLY:HA2  | 2.45                     | 0.46              |
| 1:CA:329:A:H3'     | 1:CA:330:C:C5'     | 2.45                     | 0.46              |
| 1:CA:519:C:H2'     | 1:CA:520:A:O4'     | 2.15                     | 0.46              |
| 1:CA:710:G:O2'     | 1:CA:711:G:H5'     | 2.15                     | 0.46              |
| 1:CA:756:C:H2'     | 1:CA:757:U:O4'     | 2.15                     | 0.46              |
| 2:CB:208:ILE:O     | 2:CB:212:GLN:HB2   | 2.15                     | 0.46              |
| 3:CC:52:LEU:HD12   | 3:CC:55:VAL:HG22   | 1.97                     | 0.46              |
| 4:CD:144:ASP:O     | 4:CD:184:LYS:HA    | 2.15                     | 0.46              |
| 4:CD:187:ARG:HH11  | 4:CD:187:ARG:HG2   | 1.80                     | 0.46              |
| 4:CD:23:GLY:HA3    | 4:CD:112:VAL:HG22  | 1.98                     | 0.46              |
| 7:CG:47:CYS:HB3    | 7:CG:58:PRO:CB     | 2.46                     | 0.46              |
| 11:CK:34:ASP:CB    | 11:CK:35:PRO:CD    | 2.92                     | 0.46              |
| 12:CL:58:VAL:O     | 12:CL:65:GLU:HA    | 2.16                     | 0.46              |
| 19:CS:7:LYS:HA     | 19:CS:7:LYS:HD3    | 1.72                     | 0.46              |
| 21:CU:9:ARG:HH11   | 21:CU:22:ARG:HG3   | 1.80                     | 0.46              |
| 22:CW:50:G:C2      | 22:CW:51:U:C2      | 3.03                     | 0.46              |
| 24:CY:170:ARG:O    | 24:CY:171:GLU:HG3  | 2.15                     | 0.46              |
| 24:CY:30:GLU:O     | 24:CY:31:ARG:NH1   | 2.49                     | 0.46              |
| 24:CY:491:VAL:CG1  | 24:CY:492:ASP:N    | 2.65                     | 0.46              |
| 24:CY:510:VAL:HG12 | 24:CY:511:LYS:N    | 2.30                     | 0.46              |
| 24:CY:487:ILE:CG2  | 24:CY:594:VAL:HG13 | 2.43                     | 0.46              |
| 24:CY:92:ILE:HD13  | 24:CY:93:GLU:N     | 2.31                     | 0.46              |
| 26:D1:3:LYS:HD2    | 26:D1:3:LYS:HA     | 1.67                     | 0.46              |
| 27:D2:31:GLU:HB3   | 27:D2:53:LEU:HD11  | 1.98                     | 0.46              |
| 31:D6:8:LYS:O      | 31:D6:9:LEU:O      | 2.32                     | 0.46              |
| 33:D8:48:PHE:O     | 33:D8:49:VAL:CG1   | 2.58                     | 0.46              |
| 33:D8:50:LEU:C     | 33:D8:52:LYS:H     | 2.17                     | 0.46              |
| 35:DA:1260:G:H2'   | 35:DA:1261:C:C6    | 2.49                     | 0.46              |
| 35:DA:128:C:O2'    | 35:DA:129:C:O5'    | 2.31                     | 0.46              |
| 35:DA:27:G:H1'     | 35:DA:513:A:H62    | 1.80                     | 0.46              |
| 35:DA:302:C:H2'    | 35:DA:303:U:H6     | 1.78                     | 0.46              |
| 35:DA:718:A:H3'    | 35:DA:719:C:H6     | 1.81                     | 0.46              |
| 35:DA:775:G:O6     | 35:DA:787:U:H2'    | 2.15                     | 0.46              |
| 39:DE:51:PHE:N     | 39:DE:74:PRO:HG3   | 2.30                     | 0.46              |
| 39:DE:31:CYS:C     | 39:DE:90:THR:HG23  | 2.35                     | 0.46              |
| 40:DF:126:VAL:HG23 | 40:DF:127:GLU:N    | 2.31                     | 0.46              |
| 40:DF:2:LYS:CG     | 40:DF:25:PRO:HG2   | 2.45                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 41:DG:20:ILE:O     | 41:DG:24:GLY:N      | 2.48                     | 0.46              |
| 43:DJ:103:UNK:HA   | 43:DJ:111:UNK:CB    | 2.45                     | 0.46              |
| 47:DO:69:ILE:HB    | 47:DO:77:ILE:HG22   | 1.98                     | 0.46              |
| 35:DA:2406:U:C2    | 48:DP:72:PRO:HB2    | 2.50                     | 0.46              |
| 51:DS:70:GLY:CA    | 51:DS:101:LEU:HD23  | 2.46                     | 0.46              |
| 56:DX:90:GLU:HA    | 56:DX:93:GLU:HG2    | 1.97                     | 0.46              |
| 57:DY:38:ILE:CG2   | 57:DY:39:VAL:N      | 2.78                     | 0.46              |
| 1:AA:1047:G:O2'    | 1:AA:1048:G:H5'     | 2.15                     | 0.46              |
| 1:AA:1321:C:C5'    | 1:AA:1322:C:C5'     | 2.92                     | 0.46              |
| 1:AA:218:C:H5'     | 1:AA:470:C:H41      | 1.78                     | 0.46              |
| 1:AA:756:C:H2'     | 1:AA:757:U:O4'      | 2.16                     | 0.46              |
| 2:AB:53:ARG:HG2    | 2:AB:53:ARG:O       | 2.15                     | 0.46              |
| 3:AC:60:ALA:O      | 3:AC:61:ALA:HB2     | 2.16                     | 0.46              |
| 9:AI:79:LEU:HD13   | 9:AI:83:ARG:CB      | 2.41                     | 0.46              |
| 12:AL:47:LYS:HB3   | 12:AL:47:LYS:NZ     | 2.31                     | 0.46              |
| 22:AW:74:A:H2'     | 22:AW:75:C:C5'      | 2.46                     | 0.46              |
| 23:AX:16:A:O2'     | 23:AX:17:U:H5'      | 2.16                     | 0.46              |
| 24:AY:196:ILE:CG1  | 24:AY:197:ARG:H     | 2.29                     | 0.46              |
| 26:B1:60:PHE:O     | 26:B1:62:VAL:HG12   | 2.15                     | 0.46              |
| 29:B4:37:SER:OG    | 41:BG:108:ASN:HA    | 2.15                     | 0.46              |
| 30:B5:44:THR:HG21  | 50:BR:101:ALA:CB    | 2.30                     | 0.46              |
| 31:B6:45:LYS:HG2   | 35:BA:2371:G:C4'    | 2.46                     | 0.46              |
| 31:B6:54:ILE:O     | 31:B6:54:ILE:CG1    | 2.63                     | 0.46              |
| 33:B8:53:PRO:HG2   | 33:B8:54:GLU:H      | 1.80                     | 0.46              |
| 35:BA:1061:U:C4'   | 35:BA:1070:A:H1'    | 2.43                     | 0.46              |
| 35:BA:1097:U:C2'   | 35:BA:1098:A:H5'    | 2.46                     | 0.46              |
| 35:BA:1688:U:O2    | 35:BA:1700:A:H5''   | 2.15                     | 0.46              |
| 35:BA:177:G:H3'    | 35:BA:178:G:C8      | 2.51                     | 0.46              |
| 35:BA:1813:G:H1'   | 38:BD:50:THR:OG1    | 2.15                     | 0.46              |
| 35:BA:2137:C:H2'   | 35:BA:2138:C:C6     | 2.50                     | 0.46              |
| 35:BA:2384:G:H2'   | 35:BA:2386:C:OP1    | 2.16                     | 0.46              |
| 33:B8:28:GLY:H     | 35:BA:2393:A:P      | 2.39                     | 0.46              |
| 35:BA:2454:G:H2'   | 35:BA:2455:G:H5'    | 1.97                     | 0.46              |
| 35:BA:271(M):G:H2' | 35:BA:271(N):U:H5'' | 1.98                     | 0.46              |
| 35:BA:2745:C:C4    | 35:BA:2746:U:C4     | 3.04                     | 0.46              |
| 35:BA:324:A:OP2    | 35:BA:1205:U:N3     | 2.48                     | 0.46              |
| 35:BA:438:G:H2'    | 35:BA:440:G:H8      | 1.80                     | 0.46              |
| 35:BA:784:A:H5''   | 38:BD:227:ASN:HD21  | 1.80                     | 0.46              |
| 35:BA:963:U:H2'    | 35:BA:964:C:C6      | 2.51                     | 0.46              |
| 38:BD:205:VAL:O    | 38:BD:206:LEU:C     | 2.54                     | 0.46              |
| 38:BD:48:ARG:NH1   | 38:BD:48:ARG:HG3    | 2.31                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 39:BE:31:CYS:C     | 39:BE:90:THR:HG23 | 2.36                     | 0.46              |
| 39:BE:36:ARG:HH22  | 39:BE:88:GLY:H    | 1.64                     | 0.46              |
| 39:BE:55:ASN:C     | 39:BE:57:LYS:H    | 2.17                     | 0.46              |
| 39:BE:87:GLU:O     | 39:BE:88:GLY:C    | 2.53                     | 0.46              |
| 40:BF:74:ARG:O     | 40:BF:75:HIS:CG   | 2.68                     | 0.46              |
| 42:BH:53:GLU:CD    | 42:BH:54:ARG:H    | 2.19                     | 0.46              |
| 47:BO:60:ALA:CA    | 47:BO:87:ILE:HD11 | 2.45                     | 0.46              |
| 48:BP:32:THR:CG2   | 48:BP:37:GLY:HA2  | 2.45                     | 0.46              |
| 49:BQ:109:VAL:HG12 | 49:BQ:113:GLN:HB2 | 1.98                     | 0.46              |
| 49:BQ:55:VAL:CG1   | 49:BQ:56:ARG:H    | 2.29                     | 0.46              |
| 50:BR:10:LEU:CD2   | 50:BR:17:ARG:HD3  | 2.43                     | 0.46              |
| 52:BT:83:ILE:CG1   | 52:BT:84:GLN:N    | 2.75                     | 0.46              |
| 54:BV:47:VAL:O     | 54:BV:48:GLY:C    | 2.54                     | 0.46              |
| 54:BV:64:HIS:ND1   | 54:BV:92:THR:CG2  | 2.79                     | 0.46              |
| 56:BX:3:THR:O      | 56:BX:4:ALA:HB3   | 2.15                     | 0.46              |
| 57:BY:38:ILE:CG2   | 57:BY:39:VAL:N    | 2.78                     | 0.46              |
| 1:CA:1065:U:C2'    | 1:CA:1066:C:OP2   | 2.63                     | 0.46              |
| 1:CA:608:A:C2'     | 1:CA:609:A:H5'    | 2.46                     | 0.46              |
| 1:CA:651:C:H2'     | 1:CA:652:U:H6     | 1.80                     | 0.46              |
| 1:CA:829:G:O2'     | 1:CA:830:G:H5'    | 2.15                     | 0.46              |
| 2:CB:83:MET:CG     | 2:CB:234:PRO:HG3  | 2.44                     | 0.46              |
| 3:CC:114:PRO:O     | 3:CC:118:GLN:OE1  | 2.34                     | 0.46              |
| 5:CE:76:ILE:CG1    | 5:CE:77:PRO:HD2   | 2.45                     | 0.46              |
| 9:CI:118:LYS:O     | 9:CI:119:ALA:HB3  | 2.15                     | 0.46              |
| 9:CI:70:LYS:O      | 9:CI:74:ILE:HG13  | 2.16                     | 0.46              |
| 13:CM:19:LEU:HD22  | 13:CM:19:LEU:N    | 2.29                     | 0.46              |
| 1:CA:1320:C:N4     | 19:CS:36:ARG:HG3  | 2.30                     | 0.46              |
| 20:CT:93:GLU:OE1   | 20:CT:94:ALA:N    | 2.49                     | 0.46              |
| 24:CY:420:ASP:OD2  | 24:CY:420:ASP:N   | 2.48                     | 0.46              |
| 24:CY:427:ALA:O    | 24:CY:431:LEU:HB2 | 2.16                     | 0.46              |
| 25:D0:34:GLY:O     | 25:D0:35:ASN:C    | 2.54                     | 0.46              |
| 25:D0:37:LEU:HG    | 25:D0:60:PHE:HA   | 1.98                     | 0.46              |
| 26:D1:76:ARG:CZ    | 26:D1:95:LEU:HD22 | 2.45                     | 0.46              |
| 30:D5:39:MET:HG3   | 55:DW:34:ASN:ND2  | 2.31                     | 0.46              |
| 31:D6:6:ARG:C      | 31:D6:7:ILE:CD1   | 2.83                     | 0.46              |
| 33:D8:6:THR:HG21   | 33:D8:63:PRO:HD3  | 1.98                     | 0.46              |
| 35:DA:1494:A:O2'   | 35:DA:1495:A:C5'  | 2.53                     | 0.46              |
| 35:DA:2820:A:C8    | 39:DE:191:PRO:CB  | 2.99                     | 0.46              |
| 35:DA:2840:C:H5''  | 50:DR:53:HIS:CD2  | 2.51                     | 0.46              |
| 35:DA:360:G:H2'    | 35:DA:361:G:H8    | 1.81                     | 0.46              |
| 35:DA:519:U:O2'    | 35:DA:520:G:H5'   | 2.16                     | 0.46              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:DA:63:U:H4'    | 35:DA:63:U:OP1     | 2.16                     | 0.46              |
| 35:DA:817:C:H2'   | 35:DA:818:G:O4'    | 2.15                     | 0.46              |
| 36:DB:15:A:H1'    | 36:DB:110:G:C5     | 2.51                     | 0.46              |
| 37:DC:191:ARG:HG3 | 37:DC:191:ARG:NH1  | 2.29                     | 0.46              |
| 37:DC:29:LEU:O    | 37:DC:32:GLU:N     | 2.41                     | 0.46              |
| 38:DD:31:LYS:HZ1  | 38:DD:33:LEU:HB2   | 1.79                     | 0.46              |
| 39:DE:59:VAL:CG2  | 39:DE:63:LEU:HA    | 2.46                     | 0.46              |
| 39:DE:68:ALA:HB3  | 39:DE:69:LYS:HE2   | 1.97                     | 0.46              |
| 42:DH:20:ALA:CB   | 42:DH:21:PRO:CD    | 2.90                     | 0.46              |
| 48:DP:32:THR:HG22 | 48:DP:37:GLY:HA2   | 1.98                     | 0.46              |
| 52:DT:116:ALA:HB1 | 52:DT:121:ILE:HD11 | 1.98                     | 0.46              |
| 53:DU:113:ALA:O   | 53:DU:115:ALA:N    | 2.48                     | 0.46              |
| 35:DA:997:G:OP1   | 53:DU:93:LYS:HD3   | 2.15                     | 0.46              |
| 57:DY:54:LYS:HZ3  | 57:DY:55:TYR:HE2   | 1.62                     | 0.46              |
| 58:DZ:163:LEU:HG  | 58:DZ:163:LEU:O    | 2.16                     | 0.46              |
| 1:AA:1003:G:H1'   | 1:AA:1039:C:O2     | 2.16                     | 0.46              |
| 1:AA:1253:G:C2    | 1:AA:1254:C:C2     | 3.04                     | 0.46              |
| 1:AA:1343:G:H1'   | 9:AI:121:ARG:NH1   | 2.30                     | 0.46              |
| 1:AA:1515:C:H2'   | 1:AA:1516:G:H8     | 1.79                     | 0.46              |
| 1:AA:512:U:H2'    | 1:AA:513:C:C6      | 2.47                     | 0.46              |
| 1:AA:542:G:H5'    | 4:AD:41:GLY:HA3    | 1.96                     | 0.46              |
| 4:AD:13:ARG:O     | 4:AD:14:ARG:C      | 2.53                     | 0.46              |
| 4:AD:54:TYR:O     | 4:AD:55:ALA:C      | 2.53                     | 0.46              |
| 6:AF:67:MET:CE    | 6:AF:72:VAL:HA     | 2.45                     | 0.46              |
| 9:AI:125:TYR:HD2  | 9:AI:126:SER:N     | 2.14                     | 0.46              |
| 9:AI:88:TYR:O     | 9:AI:89:ASN:CB     | 2.57                     | 0.46              |
| 10:AJ:5:ARG:HA    | 10:AJ:73:ASP:OD1   | 2.15                     | 0.46              |
| 12:AL:30:ALA:CB   | 12:AL:33:ARG:HH21  | 2.28                     | 0.46              |
| 15:AO:31:LEU:H    | 15:AO:31:LEU:CD2   | 2.28                     | 0.46              |
| 1:AA:192:U:C4'    | 20:AT:103:GLY:HA2  | 2.45                     | 0.46              |
| 20:AT:93:GLU:OE1  | 20:AT:94:ALA:N     | 2.48                     | 0.46              |
| 22:AW:59:A:H2     | 22:AW:61:U:HO2'    | 1.62                     | 0.46              |
| 24:AY:315:LYS:HZ3 | 24:AY:317:MET:HG2  | 1.80                     | 0.46              |
| 24:AY:99:ARG:CZ   | 24:AY:128:TYR:HB2  | 2.44                     | 0.46              |
| 26:B1:45:ASN:ND2  | 26:B1:47:GLN:HE21  | 2.04                     | 0.46              |
| 26:B1:94:LEU:C    | 26:B1:96:LYS:N     | 2.69                     | 0.46              |
| 31:B6:27:LYS:HB3  | 31:B6:32:ASN:HD21  | 1.74                     | 0.46              |
| 31:B6:42:TRP:CH2  | 35:BA:643:A:N7     | 2.83                     | 0.46              |
| 35:BA:1218:C:H2'  | 35:BA:1219:G:H8    | 1.79                     | 0.46              |
| 35:BA:45:C:OP2    | 35:BA:215:G:H5"    | 2.15                     | 0.46              |
| 35:BA:389:G:C6    | 48:BP:70:GLN:HG3   | 2.51                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:755:C:H2'    | 35:BA:756:C:C6     | 2.51                     | 0.46              |
| 35:BA:826:U:H5''   | 35:BA:2428:G:O3'   | 2.15                     | 0.46              |
| 37:BC:60:ARG:HG3   | 37:BC:165:ARG:HG3  | 1.96                     | 0.46              |
| 38:BD:210:GLY:O    | 38:BD:211:ARG:CB   | 2.62                     | 0.46              |
| 39:BE:101:ARG:HD3  | 39:BE:101:ARG:HA   | 1.66                     | 0.46              |
| 40:BF:24:LEU:CB    | 40:BF:25:PRO:HD2   | 2.39                     | 0.46              |
| 40:BF:36:VAL:O     | 40:BF:39:TRP:HB3   | 2.15                     | 0.46              |
| 41:BG:152:LEU:HD23 | 41:BG:152:LEU:H    | 1.79                     | 0.46              |
| 44:BK:62:ASP:O     | 44:BK:63:ARG:HB2   | 2.16                     | 0.46              |
| 46:BN:123:TYR:CD1  | 46:BN:123:TYR:N    | 2.83                     | 0.46              |
| 46:BN:99:LEU:HD13  | 46:BN:99:LEU:C     | 2.36                     | 0.46              |
| 48:BP:127:ALA:C    | 48:BP:148:LEU:HD11 | 2.36                     | 0.46              |
| 50:BR:41:ALA:C     | 50:BR:43:GLU:N     | 2.69                     | 0.46              |
| 52:BT:107:ASP:CG   | 52:BT:108:ARG:N    | 2.67                     | 0.46              |
| 52:BT:62:THR:CG2   | 52:BT:75:ILE:HG13  | 2.46                     | 0.46              |
| 1:CA:1329:A:H4'    | 13:CM:24:GLY:O     | 2.16                     | 0.46              |
| 1:CA:1416:G:H2'    | 1:CA:1417:G:C8     | 2.50                     | 0.46              |
| 1:CA:277:C:C2'     | 1:CA:278:G:H5'     | 2.46                     | 0.46              |
| 1:CA:311:C:H2'     | 1:CA:312:C:H6      | 1.81                     | 0.46              |
| 1:CA:341:C:C2      | 1:CA:349:A:C2      | 3.03                     | 0.46              |
| 1:CA:424:G:O2'     | 1:CA:425:G:H5'     | 2.16                     | 0.46              |
| 3:CC:142:MET:HE2   | 3:CC:171:GLY:CA    | 2.42                     | 0.46              |
| 3:CC:62:ASP:O      | 3:CC:64:VAL:N      | 2.48                     | 0.46              |
| 4:CD:163:GLU:C     | 4:CD:165:MET:N     | 2.69                     | 0.46              |
| 4:CD:173:TRP:O     | 4:CD:174:LEU:HD23  | 2.15                     | 0.46              |
| 5:CE:53:LEU:O      | 5:CE:56:GLN:HB3    | 2.16                     | 0.46              |
| 7:CG:84:ASN:N      | 7:CG:84:ASN:ND2    | 2.64                     | 0.46              |
| 9:CI:55:ALA:HA     | 9:CI:58:HIS:HD2    | 1.80                     | 0.46              |
| 1:CA:953:G:N7      | 13:CM:104:ARG:NH2  | 2.64                     | 0.46              |
| 13:CM:66:LEU:HA    | 13:CM:70:LEU:HD13  | 1.97                     | 0.46              |
| 18:CR:53:ARG:C     | 18:CR:55:ARG:H     | 2.17                     | 0.46              |
| 19:CS:79:THR:CG2   | 19:CS:80:TYR:N     | 2.79                     | 0.46              |
| 26:D1:46:LEU:O     | 26:D1:47:GLN:NE2   | 2.47                     | 0.46              |
| 26:D1:53:VAL:CG1   | 26:D1:90:ILE:HG21  | 2.46                     | 0.46              |
| 29:D4:35:VAL:HG12  | 29:D4:36:CYS:N     | 2.31                     | 0.46              |
| 30:D5:22:HIS:HE1   | 35:DA:2624:G:H1'   | 1.79                     | 0.46              |
| 31:D6:47:THR:OG1   | 31:D6:48:VAL:N     | 2.48                     | 0.46              |
| 35:DA:1310:G:C2'   | 35:DA:1311:G:H5'   | 2.46                     | 0.46              |
| 35:DA:1577:C:H2'   | 35:DA:1578:U:O4'   | 2.15                     | 0.46              |
| 35:DA:1771:C:H2'   | 35:DA:1772:G:C8    | 2.51                     | 0.46              |
| 35:DA:1819:A:O2'   | 35:DA:1820:U:OP2   | 2.33                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:2039:C:O2'   | 35:DA:2040:C:H5'   | 2.15                     | 0.46              |
| 35:DA:2105:C:N4    | 35:DA:2184:G:H1    | 2.12                     | 0.46              |
| 35:DA:2373:G:H2'   | 35:DA:2374:C:H6    | 1.80                     | 0.46              |
| 35:DA:2584:U:O2    | 35:DA:2584:U:O4'   | 2.33                     | 0.46              |
| 35:DA:338:G:O2'    | 35:DA:339:U:H5'    | 2.16                     | 0.46              |
| 35:DA:430:G:H2'    | 35:DA:431:U:H5'    | 1.98                     | 0.46              |
| 35:DA:586:A:C2     | 35:DA:1254:A:C2    | 3.04                     | 0.46              |
| 35:DA:797:C:H2'    | 35:DA:798:G:C8     | 2.51                     | 0.46              |
| 35:DA:94(A):G:H2'  | 35:DA:95:G:H5''    | 1.97                     | 0.46              |
| 37:DC:98:GLU:HA    | 37:DC:101:ILE:CD1  | 2.46                     | 0.46              |
| 38:DD:229:VAL:HG23 | 38:DD:230:ASP:N    | 2.31                     | 0.46              |
| 38:DD:270:ILE:H    | 38:DD:270:ILE:HD12 | 1.79                     | 0.46              |
| 39:DE:6:GLY:HA2    | 39:DE:27:LEU:O     | 2.15                     | 0.46              |
| 39:DE:38:THR:OG1   | 39:DE:41:LYS:HE2   | 2.15                     | 0.46              |
| 39:DE:92:THR:OG1   | 39:DE:95:ILE:HD11  | 2.15                     | 0.46              |
| 40:DF:160:ASN:ND2  | 40:DF:160:ASN:C    | 2.66                     | 0.46              |
| 42:DH:94:TYR:N     | 42:DH:94:TYR:CD1   | 2.84                     | 0.46              |
| 43:DJ:51:UNK:CB    | 43:DJ:89:UNK:O     | 2.63                     | 0.46              |
| 35:DA:1107:G:OP1   | 43:DJ:59:UNK:N     | 2.49                     | 0.46              |
| 48:DP:126:VAL:HG12 | 48:DP:148:LEU:HD21 | 1.98                     | 0.46              |
| 48:DP:16:ARG:HH11  | 48:DP:16:ARG:CB    | 2.28                     | 0.46              |
| 52:DT:64:ARG:HG2   | 52:DT:64:ARG:NH1   | 2.30                     | 0.46              |
| 52:DT:65:LYS:HA    | 52:DT:65:LYS:HZ2   | 1.76                     | 0.46              |
| 53:DU:90:VAL:O     | 53:DU:91:ASP:C     | 2.54                     | 0.46              |
| 54:DV:47:VAL:O     | 54:DV:48:GLY:C     | 2.54                     | 0.46              |
| 55:DW:41:LYS:C     | 55:DW:43:GLY:N     | 2.69                     | 0.46              |
| 56:DX:43:VAL:C     | 56:DX:45:THR:H     | 2.19                     | 0.46              |
| 56:DX:57:LEU:HD22  | 56:DX:57:LEU:O     | 2.15                     | 0.46              |
| 56:DX:65:ARG:HG2   | 56:DX:66:LEU:N     | 2.31                     | 0.46              |
| 57:DY:14:LEU:HD13  | 57:DY:24:VAL:CG2   | 2.46                     | 0.46              |
| 58:DZ:41:LEU:HD23  | 58:DZ:41:LEU:HA    | 1.81                     | 0.46              |
| 1:AA:1365:G:O2'    | 1:AA:1366:C:H5'    | 2.14                     | 0.46              |
| 1:AA:1500:A:OP2    | 1:AA:1505:G:OP2    | 2.33                     | 0.46              |
| 1:AA:189(A):C:H2'  | 1:AA:189(B):C:C6   | 2.51                     | 0.46              |
| 2:AB:142:LEU:CD2   | 2:AB:146:GLN:NE2   | 2.79                     | 0.46              |
| 2:AB:51:LEU:CD2    | 2:AB:201:ILE:HG23  | 2.46                     | 0.46              |
| 2:AB:95:GLN:HE21   | 2:AB:147:LYS:HE3   | 1.81                     | 0.46              |
| 5:AE:100:VAL:CG2   | 5:AE:100:VAL:O     | 2.63                     | 0.46              |
| 9:AI:114:TYR:CD2   | 9:AI:114:TYR:O     | 2.69                     | 0.46              |
| 10:AJ:54:PHE:O     | 10:AJ:55:LYS:C     | 2.53                     | 0.46              |
| 12:AL:24:VAL:O     | 12:AL:24:VAL:HG12  | 2.14                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:AL:51:ALA:O     | 12:AL:52:LEU:HD23  | 2.15                     | 0.46              |
| 1:AA:1316:G:H4'    | 14:AN:18:VAL:HG12  | 1.97                     | 0.46              |
| 20:AT:16:HIS:O     | 20:AT:17:ARG:C     | 2.54                     | 0.46              |
| 24:AY:124:GLN:O    | 24:AY:127:LYS:HB3  | 2.16                     | 0.46              |
| 24:AY:170:ARG:NH2  | 24:AY:205:TYR:HE1  | 2.13                     | 0.46              |
| 24:AY:223:PHE:CZ   | 24:AY:249:GLY:HA3  | 2.51                     | 0.46              |
| 24:AY:251:ILE:HG22 | 24:AY:251:ILE:O    | 2.14                     | 0.46              |
| 24:AY:259:PHE:C    | 24:AY:260:LEU:HD13 | 2.35                     | 0.46              |
| 24:AY:487:ILE:CD1  | 24:AY:487:ILE:H    | 2.28                     | 0.46              |
| 25:B0:40:GLN:NE2   | 25:B0:44:ARG:N     | 2.64                     | 0.46              |
| 29:B4:39:CYS:SG    | 29:B4:42:PHE:HE2   | 2.37                     | 0.46              |
| 31:B6:22:ALA:C     | 31:B6:23:THR:HG23  | 2.36                     | 0.46              |
| 33:B8:48:PHE:O     | 33:B8:49:VAL:CG2   | 2.60                     | 0.46              |
| 35:BA:1015:G:H2'   | 35:BA:1016:G:C8    | 2.51                     | 0.46              |
| 35:BA:1101:U:H2'   | 35:BA:1102:C:C6    | 2.50                     | 0.46              |
| 35:BA:1127:A:C2'   | 35:BA:1128:A:H5''  | 2.44                     | 0.46              |
| 35:BA:1166:C:H2'   | 35:BA:1167:U:H6    | 1.81                     | 0.46              |
| 26:B1:12:PRO:HG3   | 35:BA:1365:A:C5'   | 2.45                     | 0.46              |
| 35:BA:1529:G:C2    | 35:BA:1541:G:N2    | 2.84                     | 0.46              |
| 35:BA:2193:G:H8    | 35:BA:2193:G:H5'   | 1.81                     | 0.46              |
| 35:BA:2351:G:HO2'  | 35:BA:2352:A:H8    | 1.62                     | 0.46              |
| 35:BA:2481:G:O2'   | 35:BA:2482:G:P     | 2.74                     | 0.46              |
| 35:BA:512:G:HO2'   | 35:BA:513:A:H8     | 1.64                     | 0.46              |
| 35:BA:759:G:H2'    | 35:BA:760:G:C8     | 2.46                     | 0.46              |
| 36:BB:64:C:O2'     | 36:BB:65:C:H5'     | 2.15                     | 0.46              |
| 38:BD:45:ASN:HB2   | 38:BD:46:GLN:OE1   | 2.15                     | 0.46              |
| 39:BE:82:ARG:HH11  | 39:BE:82:ARG:HG3   | 1.81                     | 0.46              |
| 41:BG:31:VAL:HG22  | 41:BG:32:PRO:CD    | 2.46                     | 0.46              |
| 41:BG:97:ASP:CB    | 41:BG:98:ARG:NH1   | 2.75                     | 0.46              |
| 42:BH:33:LEU:HD21  | 42:BH:136:ILE:HG22 | 1.98                     | 0.46              |
| 46:BN:120:LEU:HD13 | 46:BN:121:LYS:N    | 2.31                     | 0.46              |
| 48:BP:144:GLU:O    | 48:BP:144:GLU:HG2  | 2.15                     | 0.46              |
| 51:BS:56:LEU:C     | 51:BS:58:LEU:H     | 2.19                     | 0.46              |
| 52:BT:82:LEU:CD2   | 52:BT:85:LYS:HD2   | 2.45                     | 0.46              |
| 52:BT:92:GLY:C     | 52:BT:94:ALA:N     | 2.69                     | 0.46              |
| 56:BX:65:ARG:HG2   | 56:BX:66:LEU:N     | 2.31                     | 0.46              |
| 1:CA:1353:G:H2'    | 1:CA:1354:C:H6     | 1.81                     | 0.46              |
| 1:CA:376:G:OP2     | 16:CP:67:THR:HG21  | 2.16                     | 0.46              |
| 1:CA:66:G:H4'      | 1:CA:173:U:H5      | 1.74                     | 0.46              |
| 3:CC:127:ARG:HG2   | 3:CC:127:ARG:HH11  | 1.81                     | 0.46              |
| 3:CC:40:ARG:HH11   | 3:CC:40:ARG:HG3    | 1.81                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:CC:83:ARG:C     | 3:CC:85:ARG:N     | 2.69                     | 0.46              |
| 5:CE:28:PHE:O     | 5:CE:47:LYS:HA    | 2.15                     | 0.46              |
| 5:CE:80:ILE:HD11  | 5:CE:138:ALA:HB1  | 1.98                     | 0.46              |
| 6:CF:15:ASP:C     | 6:CF:17:SER:H     | 2.18                     | 0.46              |
| 10:CJ:61:GLU:OE1  | 14:CN:49:HIS:CE1  | 2.62                     | 0.46              |
| 12:CL:41:ARG:CG   | 12:CL:42:THR:N    | 2.74                     | 0.46              |
| 12:CL:80:HIS:O    | 12:CL:81:SER:CB   | 2.58                     | 0.46              |
| 13:CM:23:TYR:HE1  | 13:CM:70:LEU:HD22 | 1.81                     | 0.46              |
| 19:CS:5:LEU:HG    | 19:CS:10:PHE:HD1  | 1.80                     | 0.46              |
| 20:CT:50:GLU:HB2  | 20:CT:100:ILE:HB  | 1.97                     | 0.46              |
| 22:CW:25:U:H2'    | 22:CW:26:C:H6     | 1.80                     | 0.46              |
| 22:CW:25:U:H2'    | 22:CW:26:C:O4'    | 2.15                     | 0.46              |
| 24:CY:309:LEU:HA  | 24:CY:332:SER:O   | 2.16                     | 0.46              |
| 26:D1:65:SER:O    | 26:D1:68:PRO:HD2  | 2.16                     | 0.46              |
| 31:D6:15:GLU:HG2  | 31:D6:16:CYS:O    | 2.15                     | 0.46              |
| 35:DA:1064:C:H5'' | 44:DK:86:LYS:HB2  | 1.98                     | 0.46              |
| 35:DA:1590:U:H2'  | 35:DA:1591:G:H8   | 1.80                     | 0.46              |
| 35:DA:2645:G:C3'  | 35:DA:2646:C:C5'  | 2.85                     | 0.46              |
| 35:DA:2688:U:H5   | 35:DA:2720:U:OP2  | 1.99                     | 0.46              |
| 35:DA:2740:A:C6   | 35:DA:2741:A:C6   | 3.04                     | 0.46              |
| 35:DA:389:G:C6    | 48:DP:70:GLN:HG3  | 2.51                     | 0.46              |
| 35:DA:640:C:C4    | 35:DA:641:C:N4    | 2.83                     | 0.46              |
| 35:DA:676:A:H1'   | 35:DA:2443:C:C1'  | 2.43                     | 0.46              |
| 35:DA:464:U:C4    | 35:DA:788:A:N7    | 2.84                     | 0.46              |
| 35:DA:958:U:C6    | 35:DA:958:U:H3'   | 2.50                     | 0.46              |
| 35:DA:996:A:H2'   | 35:DA:997:G:H8    | 1.80                     | 0.46              |
| 38:DD:205:VAL:O   | 38:DD:206:LEU:C   | 2.54                     | 0.46              |
| 39:DE:108:SER:O   | 39:DE:109:LYS:C   | 2.54                     | 0.46              |
| 39:DE:32:PRO:HA   | 39:DE:90:THR:HG23 | 1.97                     | 0.46              |
| 44:DK:3:LYS:HB3   | 44:DK:3:LYS:HE3   | 1.78                     | 0.46              |
| 48:DP:133:SER:O   | 48:DP:136:GLU:HG2 | 2.16                     | 0.46              |
| 49:DQ:109:VAL:CG1 | 49:DQ:113:GLN:HB2 | 2.45                     | 0.46              |
| 49:DQ:58:PHE:CD1  | 49:DQ:58:PHE:O    | 2.69                     | 0.46              |
| 52:DT:55:ASN:CG   | 52:DT:55:ASN:O    | 2.54                     | 0.46              |
| 53:DU:98:LEU:O    | 53:DU:106:PHE:HB2 | 2.16                     | 0.46              |
| 55:DW:1:MET:HE3   | 55:DW:2:GLU:H     | 1.80                     | 0.46              |
| 55:DW:82:LEU:CD1  | 55:DW:82:LEU:N    | 2.78                     | 0.46              |
| 56:DX:34:ALA:HA   | 56:DX:38:GLU:OE2  | 2.16                     | 0.46              |
| 1:AA:1221:G:H4'   | 19:AS:77:THR:CG2  | 2.39                     | 0.46              |
| 1:AA:189(C):C:H2' | 1:AA:189(D):C:O4' | 2.15                     | 0.46              |
| 1:AA:311:C:O2'    | 1:AA:312:C:H5'    | 2.16                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:328:C:O2     | 1:AA:328:C:C2'     | 2.57                     | 0.46              |
| 1:AA:509:A:H3'    | 1:AA:510:A:C8      | 2.50                     | 0.46              |
| 1:AA:930:C:C2'    | 1:AA:931:C:H5'     | 2.46                     | 0.46              |
| 1:AA:946:A:H3'    | 1:AA:947:G:H8      | 1.78                     | 0.46              |
| 1:AA:973:G:C1'    | 10:AJ:55:LYS:HE2   | 2.44                     | 0.46              |
| 3:AC:173:VAL:O    | 3:AC:175:LEU:HD12  | 2.15                     | 0.46              |
| 4:AD:159:ARG:O    | 4:AD:162:LEU:N     | 2.49                     | 0.46              |
| 8:AH:35:ILE:HG22  | 8:AH:39:LEU:HD21   | 1.98                     | 0.46              |
| 9:AI:117:HIS:O    | 9:AI:118:LYS:HG3   | 2.16                     | 0.46              |
| 10:AJ:3:LYS:N     | 10:AJ:75:ILE:O     | 2.49                     | 0.46              |
| 10:AJ:42:THR:HG23 | 10:AJ:67:THR:O     | 2.16                     | 0.46              |
| 13:AM:88:ARG:HG2  | 13:AM:88:ARG:HH11  | 1.80                     | 0.46              |
| 16:AP:8:ARG:NH2   | 16:AP:15:PRO:HG3   | 2.30                     | 0.46              |
| 16:AP:28:ARG:HG2  | 16:AP:28:ARG:NH1   | 2.31                     | 0.46              |
| 19:AS:29:ARG:HD2  | 19:AS:29:ARG:N     | 2.31                     | 0.46              |
| 20:AT:89:ARG:HD2  | 20:AT:104:LEU:HD11 | 1.98                     | 0.46              |
| 24:AY:285:ASP:OD2 | 24:AY:285:ASP:N    | 2.48                     | 0.46              |
| 24:AY:414:GLU:HA  | 24:AY:415:PRO:HD2  | 1.74                     | 0.46              |
| 24:AY:673:PHE:CG  | 24:AY:674:ASP:N    | 2.84                     | 0.46              |
| 24:AY:5:VAL:O     | 24:AY:7:TYR:N      | 2.49                     | 0.46              |
| 28:B3:43:ILE:O    | 28:B3:47:VAL:HG23  | 2.15                     | 0.46              |
| 33:B8:4:MET:SD    | 33:B8:61:LEU:HD22  | 2.56                     | 0.46              |
| 34:B9:2:LYS:HD3   | 35:BA:2526:G:N3    | 2.31                     | 0.46              |
| 35:BA:1241:A:H2'  | 35:BA:1242:A:O4'   | 2.15                     | 0.46              |
| 35:BA:1264:G:O3'  | 35:BA:2615:U:H5'   | 2.16                     | 0.46              |
| 35:BA:1464:C:O2'  | 35:BA:1528:A:C8    | 2.67                     | 0.46              |
| 35:BA:1782:C:H1'  | 35:BA:2609:U:C5'   | 2.37                     | 0.46              |
| 35:BA:1821:A:H2'  | 35:BA:1822:G:C8    | 2.51                     | 0.46              |
| 35:BA:1925:C:O2'  | 35:BA:1926:U:H5'   | 2.15                     | 0.46              |
| 35:BA:1948:G:C5'  | 35:BA:1948:G:C8    | 2.96                     | 0.46              |
| 35:BA:2075:U:C2'  | 35:BA:2076:U:H5''  | 2.46                     | 0.46              |
| 35:BA:2126:A:C4'  | 35:BA:2127:G:O5'   | 2.60                     | 0.46              |
| 35:BA:2206:G:H21  | 35:BA:2207:G:C5'   | 2.28                     | 0.46              |
| 35:BA:2809:A:OP2  | 35:BA:2891:G:N1    | 2.45                     | 0.46              |
| 35:BA:2892:A:H62  | 35:BA:2893:G:N2    | 2.13                     | 0.46              |
| 35:BA:383:U:H2'   | 35:BA:385:C:H5     | 1.80                     | 0.46              |
| 36:BB:68:C:H2'    | 36:BB:69:G:C8      | 2.48                     | 0.46              |
| 38:BD:138:VAL:HA  | 38:BD:165:ILE:HG21 | 1.98                     | 0.46              |
| 38:BD:244:ARG:HG2 | 38:BD:245:PRO:N    | 2.30                     | 0.46              |
| 38:BD:33:LEU:C    | 38:BD:33:LEU:HD23  | 2.37                     | 0.46              |
| 39:BE:199:ARG:HB2 | 39:BE:199:ARG:NH1  | 2.31                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:BF:160:ASN:HD21 | 40:BF:162:LEU:CD1  | 2.28                     | 0.46              |
| 42:BH:169:VAL:HG13 | 42:BH:170:ARG:H    | 1.80                     | 0.46              |
| 42:BH:20:ALA:CB    | 42:BH:21:PRO:CD    | 2.91                     | 0.46              |
| 35:BA:1081:U:H4'   | 44:BK:117:THR:HG21 | 1.98                     | 0.46              |
| 48:BP:122:PRO:O    | 48:BP:123:LEU:HD23 | 2.15                     | 0.46              |
| 55:BW:18:ARG:HG2   | 55:BW:18:ARG:HH11  | 1.81                     | 0.46              |
| 1:CA:114:U:H2'     | 1:CA:115:G:C8      | 2.51                     | 0.46              |
| 1:CA:1363(A):A:C4' | 1:CA:1364:U:H5''   | 2.41                     | 0.46              |
| 1:CA:1415:G:O2'    | 1:CA:1416:G:H5'    | 2.16                     | 0.46              |
| 1:CA:1420:C:O2     | 1:CA:1420:C:H2'    | 2.16                     | 0.46              |
| 1:CA:28:G:O2'      | 1:CA:296:U:OP1     | 2.33                     | 0.46              |
| 1:CA:373:A:H2'     | 1:CA:374:A:H8      | 1.81                     | 0.46              |
| 1:CA:416:G:H2'     | 1:CA:417:C:C6      | 2.51                     | 0.46              |
| 1:CA:80:G:N1       | 1:CA:90:U:H5'      | 2.31                     | 0.46              |
| 1:CA:981:U:H2'     | 1:CA:982:U:C5      | 2.50                     | 0.46              |
| 1:CA:1104:G:P      | 2:CB:111:ARG:HD2   | 2.56                     | 0.46              |
| 2:CB:235:SER:OG    | 2:CB:236:TYR:N     | 2.48                     | 0.46              |
| 3:CC:20:SER:HA     | 3:CC:57:ILE:O      | 2.15                     | 0.46              |
| 4:CD:22:LYS:O      | 4:CD:113:SER:HB3   | 2.15                     | 0.46              |
| 20:CT:53:LEU:HB3   | 20:CT:102:GLY:HA3  | 1.97                     | 0.46              |
| 1:CA:1326:C:P      | 21:CU:12:LYS:HZ2   | 2.39                     | 0.46              |
| 23:CX:12:A:C2      | 23:CX:13:A:H5'     | 2.49                     | 0.46              |
| 24:CY:260:LEU:HB2  | 24:CY:261:GLY:H    | 1.67                     | 0.46              |
| 24:CY:305:PRO:O    | 24:CY:333:GLY:HA2  | 2.16                     | 0.46              |
| 24:CY:92:ILE:HD13  | 24:CY:92:ILE:C     | 2.36                     | 0.46              |
| 24:CY:92:ILE:HB    | 24:CY:405:PRO:HG2  | 1.98                     | 0.46              |
| 26:D1:27:GLU:O     | 26:D1:28:GLY:C     | 2.54                     | 0.46              |
| 31:D6:27:LYS:HB3   | 31:D6:32:ASN:HD21  | 1.77                     | 0.46              |
| 35:DA:1050:A:C4    | 35:DA:1051:G:H1'   | 2.51                     | 0.46              |
| 35:DA:1499:C:O2'   | 35:DA:1500:G:H5'   | 2.16                     | 0.46              |
| 35:DA:1682:G:H5'   | 35:DA:1762:A:O2'   | 2.15                     | 0.46              |
| 35:DA:177:G:H3'    | 35:DA:178:G:C8     | 2.51                     | 0.46              |
| 35:DA:2206:G:H21   | 35:DA:2207:G:C5'   | 2.29                     | 0.46              |
| 35:DA:2206:G:H21   | 35:DA:2207:G:H5'   | 1.78                     | 0.46              |
| 35:DA:2286:A:H8    | 35:DA:2287:A:C6    | 2.34                     | 0.46              |
| 34:D9:6:SER:HB2    | 35:DA:2466:C:H5''  | 1.98                     | 0.46              |
| 35:DA:286:C:H2'    | 35:DA:287:C:H6     | 1.79                     | 0.46              |
| 35:DA:2892:A:H62   | 35:DA:2893:G:N2    | 2.13                     | 0.46              |
| 35:DA:803:U:H2'    | 35:DA:804:A:C5'    | 2.46                     | 0.46              |
| 35:DA:818:G:OP2    | 35:DA:1187:G:O6    | 2.34                     | 0.46              |
| 35:DA:9:U:O4       | 35:DA:2629:A:N7    | 2.49                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 37:DC:76:LEU:HD21  | 37:DC:104:ILE:CD1 | 2.46                     | 0.46              |
| 38:DD:244:ARG:HG2  | 38:DD:245:PRO:N   | 2.31                     | 0.46              |
| 39:DE:110:GLY:O    | 50:DR:2:ARG:HD3   | 2.15                     | 0.46              |
| 39:DE:107:THR:HA   | 39:DE:163:GLU:O   | 2.16                     | 0.46              |
| 39:DE:49:LEU:O     | 39:DE:78:LEU:CB   | 2.64                     | 0.46              |
| 45:DL:15:UNK:O     | 45:DL:19:UNK:N    | 2.49                     | 0.46              |
| 46:DN:15:LEU:HB2   | 46:DN:134:ARG:HB2 | 1.98                     | 0.46              |
| 49:DQ:1:MET:HE1    | 49:DQ:45:GLN:N    | 2.30                     | 0.46              |
| 50:DR:26:LYS:HE2   | 50:DR:71:GLN:H    | 1.80                     | 0.46              |
| 50:DR:44:LEU:HD13  | 50:DR:44:LEU:C    | 2.35                     | 0.46              |
| 55:DW:20:VAL:HG23  | 55:DW:21:VAL:H    | 1.80                     | 0.46              |
| 57:DY:8:LYS:HE2    | 57:DY:72:VAL:O    | 2.16                     | 0.46              |
| 1:AA:1118:C:H42    | 1:AA:1155:G:H1    | 1.63                     | 0.46              |
| 1:AA:1424:C:H2'    | 1:AA:1425:U:C6    | 2.46                     | 0.46              |
| 1:AA:324:G:N2      | 1:AA:326:G:H3'    | 2.31                     | 0.46              |
| 1:AA:416:G:H2'     | 1:AA:417:C:C6     | 2.51                     | 0.46              |
| 1:AA:46:G:O2'      | 1:AA:365:U:H1'    | 2.16                     | 0.46              |
| 1:AA:814:A:H2'     | 1:AA:816:A:C5'    | 2.42                     | 0.46              |
| 1:AA:826:C:H2'     | 1:AA:827:U:H6     | 1.79                     | 0.46              |
| 2:AB:213:LEU:C     | 2:AB:213:LEU:HD23 | 2.36                     | 0.46              |
| 2:AB:32:ILE:CD1    | 2:AB:40:HIS:HB3   | 2.45                     | 0.46              |
| 2:AB:51:LEU:HD22   | 2:AB:55:PHE:HE2   | 1.81                     | 0.46              |
| 4:AD:29:PRO:O      | 4:AD:30:LYS:CB    | 2.63                     | 0.46              |
| 8:AH:44:PHE:HE2    | 8:AH:109:ILE:CG2  | 2.28                     | 0.46              |
| 17:AQ:52:LYS:HD3   | 17:AQ:55:ASP:OD2  | 2.15                     | 0.46              |
| 20:AT:104:LEU:HD23 | 20:AT:105:SER:O   | 2.16                     | 0.46              |
| 20:AT:75:ASN:HD22  | 20:AT:75:ASN:H    | 1.63                     | 0.46              |
| 22:AV:4:G:O2'      | 22:AV:5:G:P       | 2.74                     | 0.46              |
| 22:AW:48:U:C6      | 22:AW:51:U:OP1    | 2.69                     | 0.46              |
| 24:AY:100:VAL:HG23 | 24:AY:329:ARG:CG  | 2.44                     | 0.46              |
| 24:AY:363:ARG:NH1  | 24:AY:363:ARG:HG3 | 2.23                     | 0.46              |
| 24:AY:689:LYS:CG   | 24:AY:690:GLY:N   | 2.78                     | 0.46              |
| 24:AY:76:ASP:O     | 24:AY:77:HIS:CG   | 2.68                     | 0.46              |
| 25:B0:19:LYS:HD3   | 25:B0:41:ARG:NH2  | 2.26                     | 0.46              |
| 26:B1:44:PRO:HB2   | 26:B1:46:LEU:CD1  | 2.46                     | 0.46              |
| 26:B1:92:LYS:CE    | 35:BA:153:C:OP1   | 2.64                     | 0.46              |
| 31:B6:43:CYS:CB    | 31:B6:44:ARG:HH21 | 2.23                     | 0.46              |
| 34:B9:3:VAL:O      | 34:B9:4:ARG:HB3   | 2.16                     | 0.46              |
| 35:BA:1159:U:H5''  | 35:BA:1159:U:H6   | 1.81                     | 0.46              |
| 35:BA:1196:C:O2'   | 35:BA:1197:G:H5'  | 2.16                     | 0.46              |
| 35:BA:1491:G:H21   | 35:BA:1492:G:H1'  | 1.81                     | 0.46              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:2105:C:N4    | 35:BA:2184:G:H1    | 2.12                     | 0.46              |
| 35:BA:2307:G:H3'   | 35:BA:2308:G:C5'   | 2.45                     | 0.46              |
| 35:BA:324:A:N6     | 35:BA:338:G:O2'    | 2.49                     | 0.46              |
| 35:BA:393:C:O2'    | 35:BA:394:A:H5'    | 2.14                     | 0.46              |
| 35:BA:428:A:H3'    | 35:BA:429:A:H8     | 1.80                     | 0.46              |
| 35:BA:71:A:N3      | 35:BA:73:A:N6      | 2.64                     | 0.46              |
| 38:BD:45:ASN:CG    | 38:BD:46:GLN:H     | 2.19                     | 0.46              |
| 39:BE:59:VAL:CG2   | 39:BE:63:LEU:HA    | 2.45                     | 0.46              |
| 40:BF:4:VAL:HA     | 40:BF:19:GLU:HB3   | 1.96                     | 0.46              |
| 43:BJ:108:UNK:O    | 43:BJ:109:UNK:C    | 2.64                     | 0.46              |
| 1:AA:1423:G:H5''   | 47:BO:49:ARG:HH22  | 1.81                     | 0.46              |
| 47:BO:9:GLU:O      | 47:BO:83:ALA:HA    | 2.15                     | 0.46              |
| 48:BP:71:VAL:HG12  | 48:BP:72:PRO:HD3   | 1.97                     | 0.46              |
| 50:BR:63:ARG:HA    | 50:BR:80:PHE:CZ    | 2.51                     | 0.46              |
| 52:BT:11:GLU:C     | 52:BT:13:ARG:N     | 2.70                     | 0.46              |
| 52:BT:26:ASP:OD2   | 52:BT:26:ASP:O     | 2.34                     | 0.46              |
| 57:BY:74:PRO:HG3   | 57:BY:83:THR:CG2   | 2.45                     | 0.46              |
| 58:BZ:153:SER:O    | 58:BZ:155:LEU:HD23 | 2.15                     | 0.46              |
| 1:CA:1053:G:C4'    | 1:CA:1054:C:H5'    | 2.46                     | 0.46              |
| 1:CA:961:U:OP2     | 1:CA:1223:C:C4'    | 2.64                     | 0.46              |
| 2:CB:189:ASP:C     | 2:CB:191:ASP:H     | 2.17                     | 0.46              |
| 2:CB:238:LEU:O     | 2:CB:240:GLN:N     | 2.49                     | 0.46              |
| 5:CE:150:ARG:O     | 5:CE:150:ARG:HG2   | 2.16                     | 0.46              |
| 8:CH:19:VAL:HG23   | 8:CH:21:LYS:HB2    | 1.97                     | 0.46              |
| 9:CI:9:ARG:HB3     | 9:CI:104:ARG:HH12  | 1.81                     | 0.46              |
| 12:CL:117:ARG:HH22 | 12:CL:124:LYS:HB2  | 1.81                     | 0.46              |
| 13:CM:4:ILE:CG2    | 13:CM:5:ALA:H      | 2.25                     | 0.46              |
| 18:CR:59:SER:N     | 18:CR:62:GLU:HB2   | 2.24                     | 0.46              |
| 24:CY:394:ALA:HB1  | 24:CY:395:PRO:HD2  | 1.97                     | 0.46              |
| 24:CY:81:ILE:C     | 24:CY:82:ILE:HG13  | 2.36                     | 0.46              |
| 25:D0:40:GLN:NE2   | 25:D0:44:ARG:N     | 2.64                     | 0.46              |
| 28:D3:44:ARG:O     | 28:D3:45:GLY:C     | 2.54                     | 0.46              |
| 29:D4:9:LEU:HD13   | 29:D4:10:VAL:H     | 1.81                     | 0.46              |
| 35:DA:1061:U:C4'   | 35:DA:1070:A:H1'   | 2.43                     | 0.46              |
| 35:DA:1077:A:O2'   | 35:DA:1078:U:H5'   | 2.16                     | 0.46              |
| 35:DA:1109:C:O2    | 35:DA:1109:C:C2'   | 2.64                     | 0.46              |
| 35:DA:1668:A:H61   | 35:DA:1676:A:H61   | 1.63                     | 0.46              |
| 35:DA:1843:C:H2'   | 35:DA:1844:C:C6    | 2.50                     | 0.46              |
| 35:DA:7:G:H1       | 35:DA:2896:C:N4    | 2.13                     | 0.46              |
| 35:DA:325:G:H2'    | 35:DA:326:G:C8     | 2.50                     | 0.46              |
| 35:DA:512:G:HO2'   | 35:DA:513:A:H8     | 1.64                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:520:G:H2'    | 35:DA:521:G:H8     | 1.81                     | 0.46              |
| 35:DA:848:G:H5''   | 35:DA:928:G:N2     | 2.30                     | 0.46              |
| 35:DA:821:A:H2'    | 35:DA:946:G:H5''   | 1.98                     | 0.46              |
| 37:DC:150:ILE:HG13 | 37:DC:154:ILE:HG13 | 1.97                     | 0.46              |
| 38:DD:196:VAL:HG12 | 38:DD:196:VAL:O    | 2.16                     | 0.46              |
| 38:DD:70:TRP:CD1   | 38:DD:70:TRP:C     | 2.89                     | 0.46              |
| 39:DE:36:ARG:HH22  | 39:DE:88:GLY:H     | 1.64                     | 0.46              |
| 40:DF:165:ARG:HH11 | 40:DF:165:ARG:HB3  | 1.80                     | 0.46              |
| 42:DH:20:ALA:HB1   | 42:DH:21:PRO:HD3   | 1.98                     | 0.46              |
| 44:DK:99:ILE:O     | 44:DK:139:VAL:N    | 2.49                     | 0.46              |
| 35:DA:1006:C:O2'   | 46:DN:106:MET:HB3  | 2.15                     | 0.46              |
| 46:DN:129:PRO:O    | 46:DN:130:HIS:CB   | 2.59                     | 0.46              |
| 49:DQ:78:PRO:HB2   | 49:DQ:81:VAL:HG11  | 1.98                     | 0.46              |
| 50:DR:33:ARG:HG3   | 50:DR:115:GLU:HG3  | 1.98                     | 0.46              |
| 52:DT:32:TYR:HB3   | 52:DT:81:PRO:HB2   | 1.98                     | 0.46              |
| 52:DT:75:ILE:CD1   | 52:DT:75:ILE:N     | 2.77                     | 0.46              |
| 57:DY:7:VAL:HG21   | 57:DY:8:LYS:NZ     | 2.31                     | 0.46              |
| 1:AA:1198:G:C6     | 1:AA:1199:U:N3     | 2.84                     | 0.46              |
| 1:AA:1216:G:H2'    | 1:AA:1217:C:C6     | 2.51                     | 0.46              |
| 1:AA:1505:G:H4'    | 1:AA:1506:U:C5'    | 2.46                     | 0.46              |
| 1:AA:243:A:C2      | 1:AA:246:A:C8      | 3.03                     | 0.46              |
| 1:AA:473:G:H2'     | 1:AA:474:G:C8      | 2.47                     | 0.46              |
| 1:AA:781:A:C2'     | 1:AA:782:A:H5'     | 2.46                     | 0.46              |
| 1:AA:992:U:O2'     | 1:AA:993:G:P       | 2.74                     | 0.46              |
| 3:AC:20:SER:HA     | 3:AC:57:ILE:O      | 2.16                     | 0.46              |
| 5:AE:150:ARG:O     | 5:AE:150:ARG:HG2   | 2.16                     | 0.46              |
| 6:AF:21:LEU:O      | 6:AF:24:GLU:HB3    | 2.16                     | 0.46              |
| 8:AH:83:ILE:CD1    | 8:AH:137:VAL:HG22  | 2.41                     | 0.46              |
| 10:AJ:79:ARG:HA    | 10:AJ:79:ARG:HD3   | 1.62                     | 0.46              |
| 11:AK:87:THR:O     | 11:AK:88:GLY:C     | 2.54                     | 0.46              |
| 15:AO:31:LEU:N     | 15:AO:31:LEU:HD22  | 2.31                     | 0.46              |
| 20:AT:57:ARG:NH1   | 20:AT:102:GLY:CA   | 2.74                     | 0.46              |
| 22:AV:27:U:H6      | 22:AV:27:U:O5'     | 1.99                     | 0.46              |
| 24:AY:146:LEU:HD23 | 24:AY:146:LEU:C    | 2.36                     | 0.46              |
| 24:AY:168:ILE:HG22 | 24:AY:175:SER:OG   | 2.16                     | 0.46              |
| 24:AY:181:LEU:HD11 | 24:AY:242:LEU:HD22 | 1.97                     | 0.46              |
| 24:AY:70:THR:O     | 24:AY:80:ASN:HA    | 2.15                     | 0.46              |
| 26:B1:24:ALA:HA    | 26:B1:32:LYS:HG3   | 1.98                     | 0.46              |
| 26:B1:44:PRO:O     | 26:B1:46:LEU:HD13  | 2.16                     | 0.46              |
| 33:B8:56:GLU:HA    | 33:B8:59:LYS:HZ3   | 1.75                     | 0.46              |
| 34:B9:4:ARG:NH1    | 35:BA:2477:C:N4    | 2.64                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 35:BA:1109:C:C2'   | 35:BA:1109:C:O2     | 2.64                     | 0.46              |
| 35:BA:1188:U:C2'   | 35:BA:1189:A:H5'    | 2.45                     | 0.46              |
| 35:BA:2163:C:C2'   | 35:BA:2164:C:H5'    | 2.46                     | 0.46              |
| 35:BA:2478:A:C2'   | 35:BA:2479:G:H5'    | 2.46                     | 0.46              |
| 35:BA:2794:C:N4    | 35:BA:2801(A):A:H61 | 2.13                     | 0.46              |
| 35:BA:391:G:O2'    | 35:BA:392:C:H5'     | 2.15                     | 0.46              |
| 35:BA:654(P):C:O2' | 35:BA:654(Q):C:H5'  | 2.15                     | 0.46              |
| 35:BA:739:G:HO2'   | 35:BA:740:U:H6      | 1.60                     | 0.46              |
| 35:BA:911:A:H2'    | 49:BQ:9:TYR:OH      | 2.15                     | 0.46              |
| 38:BD:213:ARG:C    | 38:BD:215:LEU:N     | 2.67                     | 0.46              |
| 39:BE:49:LEU:O     | 39:BE:78:LEU:CB     | 2.64                     | 0.46              |
| 41:BG:111:LEU:CD2  | 41:BG:120:LEU:HD21  | 2.45                     | 0.46              |
| 41:BG:139:LEU:HD23 | 41:BG:149:VAL:HG11  | 1.98                     | 0.46              |
| 41:BG:7:LEU:HD11   | 41:BG:103:LEU:HB2   | 1.98                     | 0.46              |
| 42:BH:13:LYS:C     | 42:BH:15:VAL:H      | 2.17                     | 0.46              |
| 48:BP:115:LEU:HA   | 48:BP:134:ALA:CB    | 2.42                     | 0.46              |
| 35:BA:814:C:C5     | 48:BP:27:HIS:CE1    | 3.04                     | 0.46              |
| 48:BP:50:ARG:HG3   | 48:BP:51:PHE:N      | 2.31                     | 0.46              |
| 51:BS:89:ARG:HG3   | 51:BS:92:TYR:N      | 2.30                     | 0.46              |
| 52:BT:108:ARG:HH11 | 52:BT:108:ARG:HB2   | 1.79                     | 0.46              |
| 52:BT:102:ILE:HB   | 52:BT:110:ILE:CD1   | 2.45                     | 0.46              |
| 52:BT:82:LEU:N     | 52:BT:82:LEU:CD1    | 2.78                     | 0.46              |
| 53:BU:31:SER:O     | 53:BU:33:ARG:N      | 2.48                     | 0.46              |
| 56:BX:12:VAL:CB    | 56:BX:17:ALA:HB1    | 2.14                     | 0.46              |
| 57:BY:31:LEU:CD2   | 57:BY:31:LEU:N      | 2.78                     | 0.46              |
| 57:BY:8:LYS:HE2    | 57:BY:72:VAL:O      | 2.16                     | 0.46              |
| 1:CA:1003:G:HO2'   | 1:CA:1005:A:P       | 2.39                     | 0.46              |
| 1:CA:1195:C:H2'    | 1:CA:1197:G:O4'     | 2.16                     | 0.46              |
| 1:CA:1346:A:H1'    | 1:CA:1348:U:C5      | 2.51                     | 0.46              |
| 1:CA:1443:G:N3     | 1:CA:1443:G:H2'     | 2.29                     | 0.46              |
| 1:CA:221:C:H5'     | 1:CA:222:U:OP2      | 2.16                     | 0.46              |
| 2:CB:86:GLU:C      | 2:CB:88:ALA:N       | 2.69                     | 0.46              |
| 3:CC:64:VAL:HG12   | 3:CC:66:VAL:HG23    | 1.98                     | 0.46              |
| 4:CD:8:VAL:C       | 4:CD:10:ARG:N       | 2.69                     | 0.46              |
| 5:CE:43:LEU:CD2    | 5:CE:132:ALA:HB1    | 2.46                     | 0.46              |
| 9:CI:111:ARG:HG2   | 9:CI:112:LYS:N      | 2.30                     | 0.46              |
| 10:CJ:3:LYS:N      | 10:CJ:75:ILE:O      | 2.49                     | 0.46              |
| 13:CM:106:ASN:HB3  | 13:CM:107:ALA:H     | 1.52                     | 0.46              |
| 15:CO:17:ARG:NH1   | 15:CO:77:ARG:NH1    | 2.64                     | 0.46              |
| 24:CY:146:LEU:CD1  | 24:CY:167:PRO:HD3   | 2.46                     | 0.46              |
| 24:CY:238:THR:HG23 | 24:CY:241:GLU:N     | 2.24                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:CY:276:VAL:CA   | 24:CY:280:LEU:HD23 | 2.46                     | 0.46              |
| 24:CY:428:LEU:HD13 | 24:CY:440:VAL:HG11 | 1.96                     | 0.46              |
| 24:CY:484:ARG:CD   | 24:CY:559:PRO:HB2  | 2.46                     | 0.46              |
| 27:D2:45:SER:O     | 27:D2:46:GLN:NE2   | 2.49                     | 0.46              |
| 31:D6:45:LYS:HG2   | 35:DA:2371:G:C4'   | 2.46                     | 0.46              |
| 31:D6:7:ILE:CD1    | 31:D6:7:ILE:N      | 2.79                     | 0.46              |
| 33:D8:36:LYS:O     | 33:D8:37:SER:C     | 2.54                     | 0.46              |
| 35:DA:1022:G:O2'   | 35:DA:1023:U:P     | 2.74                     | 0.46              |
| 35:DA:1141:U:OP1   | 46:DN:25:ARG:NH1   | 2.49                     | 0.46              |
| 35:DA:120:U:O2     | 35:DA:120:U:C2'    | 2.62                     | 0.46              |
| 35:DA:1596:A:C2'   | 35:DA:1597:A:H5'   | 2.45                     | 0.46              |
| 35:DA:1808:U:H2'   | 35:DA:1809:A:O4'   | 2.16                     | 0.46              |
| 35:DA:1812:A:O2'   | 35:DA:1813:G:H5'   | 2.16                     | 0.46              |
| 35:DA:1930:G:O2'   | 35:DA:1931:U:O5'   | 2.34                     | 0.46              |
| 35:DA:20:C:H2'     | 35:DA:21:A:C8      | 2.51                     | 0.46              |
| 35:DA:186:G:C2     | 35:DA:211:A:C2     | 3.04                     | 0.46              |
| 35:DA:211:A:H2'    | 35:DA:212:G:C5'    | 2.23                     | 0.46              |
| 35:DA:2228:G:H2'   | 35:DA:2229:C:H6    | 1.76                     | 0.46              |
| 35:DA:2314:C:C2'   | 35:DA:2315:G:H5'   | 2.46                     | 0.46              |
| 33:D8:42:ARG:HH11  | 35:DA:2350:C:H5    | 1.64                     | 0.46              |
| 35:DA:2428:G:H5'   | 35:DA:2429:G:P     | 2.56                     | 0.46              |
| 35:DA:2859:G:H2'   | 35:DA:2860:A:C8    | 2.51                     | 0.46              |
| 35:DA:288:C:O2'    | 35:DA:289:A:H5'    | 2.16                     | 0.46              |
| 35:DA:343:C:O2'    | 35:DA:344:G:H5'    | 2.15                     | 0.46              |
| 32:D7:5:TRP:CZ3    | 35:DA:464:U:H4'    | 2.51                     | 0.46              |
| 35:DA:492:A:O2'    | 35:DA:493:G:H5'    | 2.16                     | 0.46              |
| 35:DA:773:U:H2'    | 35:DA:774:A:H5'    | 1.98                     | 0.46              |
| 35:DA:814:C:C5     | 48:DP:27:HIS:CE1   | 3.04                     | 0.46              |
| 35:DA:841:A:H2'    | 35:DA:842:G:O4'    | 2.15                     | 0.46              |
| 35:DA:859:G:N2     | 35:DA:917:A:OP2    | 2.27                     | 0.46              |
| 37:DC:85:LYS:O     | 37:DC:89:GLU:HG3   | 2.16                     | 0.46              |
| 38:DD:139:GLY:H    | 38:DD:165:ILE:HB   | 1.80                     | 0.46              |
| 38:DD:147:LEU:HD12 | 38:DD:147:LEU:HA   | 1.66                     | 0.46              |
| 38:DD:227:ASN:O    | 38:DD:230:ASP:N    | 2.45                     | 0.46              |
| 38:DD:270:ILE:H    | 38:DD:270:ILE:CD1  | 2.28                     | 0.46              |
| 38:DD:35:LYS:HD2   | 38:DD:36:PRO:HA    | 1.96                     | 0.46              |
| 42:DH:66:GLY:HA2   | 42:DH:69:ARG:CB    | 2.43                     | 0.46              |
| 44:DK:103:GLN:C    | 44:DK:106:GLU:HG2  | 2.36                     | 0.46              |
| 44:DK:17:ALA:HB3   | 44:DK:38:VAL:CG1   | 2.46                     | 0.46              |
| 48:DP:77:ARG:HB2   | 48:DP:78:PRO:CD    | 2.40                     | 0.46              |
| 50:DR:83:ILE:O     | 50:DR:87:TYR:CE2   | 2.69                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 52:DT:128:GLU:OE2  | 52:DT:129:ARG:N   | 2.49                     | 0.46              |
| 54:DV:35:LEU:HB3   | 54:DV:37:VAL:HG23 | 1.98                     | 0.46              |
| 57:DY:52:SER:N     | 57:DY:53:PRO:HD2  | 2.30                     | 0.46              |
| 57:DY:74:PRO:HG3   | 57:DY:83:THR:CG2  | 2.45                     | 0.46              |
| 58:DZ:56:VAL:HA    | 58:DZ:70:LEU:HD23 | 1.98                     | 0.46              |
| 1:AA:1053:G:C4'    | 1:AA:1054:C:H5'   | 2.45                     | 0.45              |
| 1:AA:1410:G:H2'    | 1:AA:1411:C:C6    | 2.50                     | 0.45              |
| 1:AA:252:U:C4      | 1:AA:253:U:O4     | 2.70                     | 0.45              |
| 1:AA:335:C:O2'     | 1:AA:336:C:H5'    | 2.16                     | 0.45              |
| 1:AA:545:C:O2'     | 1:AA:546:G:H5'    | 2.16                     | 0.45              |
| 1:AA:830:G:H2'     | 1:AA:831:U:C6     | 2.52                     | 0.45              |
| 2:AB:119:GLU:C     | 2:AB:121:LEU:H    | 2.20                     | 0.45              |
| 3:AC:206:GLU:HG2   | 3:AC:207:VAL:N    | 2.30                     | 0.45              |
| 3:AC:43:LEU:HD22   | 3:AC:47:LEU:HD22  | 1.98                     | 0.45              |
| 11:AK:125:PHE:N    | 11:AK:125:PHE:HD1 | 2.14                     | 0.45              |
| 14:AN:42:ILE:HA    | 14:AN:42:ILE:HD13 | 1.68                     | 0.45              |
| 15:AO:31:LEU:CD2   | 15:AO:31:LEU:N    | 2.79                     | 0.45              |
| 16:AP:59:TRP:O     | 16:AP:62:VAL:HG22 | 2.16                     | 0.45              |
| 16:AP:74:LEU:HD22  | 16:AP:79:VAL:HG21 | 1.98                     | 0.45              |
| 24:AY:150:ILE:C    | 24:AY:152:THR:N   | 2.69                     | 0.45              |
| 24:AY:526:VAL:N    | 24:AY:565:VAL:O   | 2.49                     | 0.45              |
| 29:B4:14:ILE:O     | 29:B4:15:ILE:HD13 | 2.16                     | 0.45              |
| 29:B4:7:PRO:HG2    | 41:BG:61:ALA:O    | 2.16                     | 0.45              |
| 31:B6:12:GLU:HA    | 31:B6:23:THR:HA   | 1.99                     | 0.45              |
| 35:BA:818:G:OP2    | 35:BA:1187:G:O6   | 2.34                     | 0.45              |
| 35:BA:1607:C:H5'   | 35:BA:1608:A:C8   | 2.51                     | 0.45              |
| 35:BA:1788:C:H2'   | 35:BA:1789:A:C8   | 2.50                     | 0.45              |
| 35:BA:2313:C:O2'   | 35:BA:2314:C:H5'  | 2.16                     | 0.45              |
| 35:BA:2722:G:O2'   | 50:BR:5:LYS:HB2   | 2.16                     | 0.45              |
| 35:BA:2732:G:H5''  | 35:BA:2733:A:C8   | 2.52                     | 0.45              |
| 35:BA:2807:G:H3'   | 35:BA:2808:U:C5'  | 2.39                     | 0.45              |
| 35:BA:539:G:O2'    | 35:BA:540:C:H5'   | 2.17                     | 0.45              |
| 35:BA:560:C:H2'    | 35:BA:561:G:O4'   | 2.16                     | 0.45              |
| 35:BA:676:A:H1'    | 35:BA:2443:C:C1'  | 2.43                     | 0.45              |
| 35:BA:725:G:C6     | 35:BA:726:G:N1    | 2.84                     | 0.45              |
| 35:BA:925:C:C4     | 35:BA:926:A:N7    | 2.84                     | 0.45              |
| 35:BA:962:G:C2'    | 35:BA:963:U:H5'   | 2.45                     | 0.45              |
| 36:BB:15:A:H1'     | 36:BB:110:G:C5    | 2.50                     | 0.45              |
| 38:BD:11:PRO:C     | 38:BD:13:ARG:N    | 2.68                     | 0.45              |
| 41:BG:152:LEU:HD23 | 41:BG:152:LEU:N   | 2.30                     | 0.45              |
| 46:BN:32:THR:HG23  | 46:BN:37:LYS:HB3  | 1.99                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:BO:69:ILE:HD12  | 47:BO:69:ILE:H     | 1.79                     | 0.45              |
| 35:BA:626:U:H3     | 48:BP:105:LEU:HG   | 1.81                     | 0.45              |
| 35:BA:661:C:H4'    | 48:BP:18:ARG:HG2   | 1.97                     | 0.45              |
| 52:BT:102:ILE:HG13 | 52:BT:103:ARG:N    | 2.31                     | 0.45              |
| 52:BT:33:LYS:NZ    | 52:BT:43:GLN:NE2   | 2.65                     | 0.45              |
| 53:BU:50:ARG:C     | 53:BU:52:ARG:N     | 2.68                     | 0.45              |
| 53:BU:72:HIS:HE1   | 53:BU:107:ALA:HB2  | 1.82                     | 0.45              |
| 54:BV:21:ARG:HB3   | 54:BV:91:TYR:HD1   | 1.71                     | 0.45              |
| 54:BV:35:LEU:C     | 54:BV:37:VAL:H     | 2.19                     | 0.45              |
| 54:BV:39:LEU:O     | 54:BV:40:LEU:CB    | 2.64                     | 0.45              |
| 54:BV:89:GLN:OE1   | 54:BV:89:GLN:HA    | 2.17                     | 0.45              |
| 35:BA:1614:A:H62   | 55:BW:93:ALA:HB2   | 1.81                     | 0.45              |
| 58:BZ:27:VAL:O     | 58:BZ:27:VAL:HG13  | 2.17                     | 0.45              |
| 1:CA:1094:G:O2'    | 1:CA:1095:U:OP2    | 2.34                     | 0.45              |
| 1:CA:1431:C:H2'    | 1:CA:1432:G:H5'    | 1.98                     | 0.45              |
| 1:CA:311:C:O2'     | 1:CA:312:C:H5'     | 2.17                     | 0.45              |
| 1:CA:534:U:H6      | 1:CA:534:U:H5'     | 1.81                     | 0.45              |
| 1:CA:724:G:O2'     | 1:CA:725:G:H5'     | 2.16                     | 0.45              |
| 2:CB:113:HIS:O     | 2:CB:117:GLU:HG3   | 2.16                     | 0.45              |
| 2:CB:17:PHE:CG     | 2:CB:18:GLY:N      | 2.83                     | 0.45              |
| 2:CB:8:LYS:HB2     | 2:CB:9:GLU:OE2     | 2.16                     | 0.45              |
| 3:CC:138:VAL:O     | 3:CC:140:ARG:N     | 2.49                     | 0.45              |
| 5:CE:101:ILE:N     | 5:CE:101:ILE:HD13  | 2.20                     | 0.45              |
| 6:CF:97:PHE:O      | 18:CR:31:LEU:HD23  | 2.17                     | 0.45              |
| 8:CH:6:ILE:HG21    | 8:CH:85:ARG:NH1    | 2.30                     | 0.45              |
| 9:CI:126:SER:O     | 9:CI:127:LYS:HB3   | 2.16                     | 0.45              |
| 9:CI:33:PHE:C      | 9:CI:35:GLU:H      | 2.19                     | 0.45              |
| 12:CL:115:LYS:O    | 12:CL:117:ARG:N    | 2.48                     | 0.45              |
| 1:CA:190:U:O2      | 20:CT:105:SER:HB2  | 2.16                     | 0.45              |
| 24:CY:170:ARG:HH22 | 24:CY:205:TYR:HE1  | 1.62                     | 0.45              |
| 24:CY:456:GLU:O    | 24:CY:459:LEU:HD12 | 2.16                     | 0.45              |
| 24:CY:568:TYR:CD2  | 24:CY:569:ASP:HB2  | 2.51                     | 0.45              |
| 27:D2:46:GLN:O     | 27:D2:47:ASN:O     | 2.33                     | 0.45              |
| 27:D2:6:VAL:HG12   | 27:D2:6:VAL:O      | 2.16                     | 0.45              |
| 30:D5:33:CYS:SG    | 30:D5:36:CYS:SG    | 3.11                     | 0.45              |
| 35:DA:1071:G:N2    | 35:DA:1090:U:C5    | 2.83                     | 0.45              |
| 35:DA:1101:U:H2'   | 35:DA:1102:C:C6    | 2.50                     | 0.45              |
| 35:DA:1355:G:O2'   | 35:DA:1356:G:H5'   | 2.15                     | 0.45              |
| 35:DA:1675:C:H2'   | 35:DA:1676:A:O4'   | 2.17                     | 0.45              |
| 35:DA:2478:A:C2'   | 35:DA:2479:G:H5'   | 2.45                     | 0.45              |
| 35:DA:2507:C:H2'   | 35:DA:2508:G:H8    | 1.81                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:DA:2543:G:C2   | 35:DA:2765:A:H2'   | 2.51                     | 0.45              |
| 35:DA:2573:C:OP1  | 35:DA:2574:G:OP1   | 2.34                     | 0.45              |
| 35:DA:1462:C:H4'  | 35:DA:2703:C:H5'   | 1.98                     | 0.45              |
| 35:DA:2776:A:C6   | 35:DA:2782:G:H1'   | 2.50                     | 0.45              |
| 35:DA:2809:A:OP2  | 35:DA:2891:G:N1    | 2.46                     | 0.45              |
| 35:DA:311:A:H5'   | 35:DA:332:A:N3     | 2.31                     | 0.45              |
| 35:DA:777:A:C2    | 35:DA:778:G:C4     | 3.03                     | 0.45              |
| 35:DA:911:A:H2'   | 49:DQ:9:TYR:OH     | 2.16                     | 0.45              |
| 35:DA:1843:C:H5'  | 38:DD:253:GLN:NE2  | 2.30                     | 0.45              |
| 38:DD:35:LYS:CG   | 38:DD:63:ARG:HA    | 2.33                     | 0.45              |
| 39:DE:120:TRP:CE3 | 39:DE:155:LYS:HE3  | 2.51                     | 0.45              |
| 39:DE:174:ASP:OD2 | 39:DE:175:VAL:N    | 2.49                     | 0.45              |
| 39:DE:199:ARG:NH1 | 39:DE:199:ARG:HB2  | 2.32                     | 0.45              |
| 41:DG:31:VAL:HG13 | 41:DG:31:VAL:O     | 2.15                     | 0.45              |
| 41:DG:47:LYS:HD3  | 41:DG:47:LYS:H     | 1.81                     | 0.45              |
| 42:DH:53:GLU:CD   | 42:DH:54:ARG:H     | 2.19                     | 0.45              |
| 44:DK:106:GLU:HG3 | 44:DK:107:ILE:N    | 2.30                     | 0.45              |
| 46:DN:119:ARG:HG3 | 46:DN:119:ARG:HH11 | 1.81                     | 0.45              |
| 46:DN:123:TYR:N   | 46:DN:123:TYR:CD1  | 2.84                     | 0.45              |
| 47:DO:24:VAL:O    | 47:DO:24:VAL:HG23  | 2.14                     | 0.45              |
| 48:DP:32:THR:CG2  | 48:DP:37:GLY:HA2   | 2.45                     | 0.45              |
| 48:DP:46:LYS:HG2  | 48:DP:52:GLU:CG    | 2.46                     | 0.45              |
| 48:DP:98:GLU:O    | 48:DP:102:ARG:NH2  | 2.49                     | 0.45              |
| 51:DS:106:ARG:O   | 51:DS:107:GLU:HB2  | 2.15                     | 0.45              |
| 51:DS:35:ILE:HD11 | 51:DS:99:LYS:HE3   | 1.98                     | 0.45              |
| 51:DS:44:LYS:O    | 51:DS:46:VAL:HG23  | 2.16                     | 0.45              |
| 53:DU:49:HIS:O    | 53:DU:52:ARG:HB2   | 2.16                     | 0.45              |
| 54:DV:39:LEU:HA   | 54:DV:47:VAL:CG1   | 2.45                     | 0.45              |
| 35:DA:1187:G:H5'' | 54:DV:81:TYR:CE2   | 2.51                     | 0.45              |
| 55:DW:12:ILE:HG13 | 55:DW:42:ARG:NH1   | 2.31                     | 0.45              |
| 56:DX:3:THR:O     | 56:DX:4:ALA:HB3    | 2.17                     | 0.45              |
| 58:DZ:168:GLU:HG3 | 58:DZ:169:GLU:N    | 2.31                     | 0.45              |
| 1:AA:1169:A:H2'   | 1:AA:1170:A:C8     | 2.51                     | 0.45              |
| 1:AA:1234:C:HO2'  | 1:AA:1364:U:H6     | 1.61                     | 0.45              |
| 1:AA:1371:G:C6    | 1:AA:1372:U:C4     | 3.03                     | 0.45              |
| 1:AA:470:C:C2'    | 1:AA:471:G:OP1     | 2.64                     | 0.45              |
| 1:AA:896:C:O2'    | 1:AA:897:C:H5'     | 2.17                     | 0.45              |
| 2:AB:179:LYS:O    | 2:AB:179:LYS:HG2   | 2.16                     | 0.45              |
| 3:AC:131:ARG:O    | 3:AC:132:ARG:C     | 2.54                     | 0.45              |
| 3:AC:151:VAL:CG1  | 3:AC:152:ILE:N     | 2.79                     | 0.45              |
| 3:AC:35:GLU:O     | 3:AC:39:ILE:HG13   | 2.16                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:AC:52:LEU:HD12   | 3:AC:55:VAL:HG22   | 1.98                     | 0.45              |
| 4:AD:159:ARG:HG3   | 4:AD:159:ARG:NH1   | 2.31                     | 0.45              |
| 1:AA:559:A:P       | 5:AE:126:ARG:HH22  | 2.39                     | 0.45              |
| 5:AE:136:MET:O     | 5:AE:137:GLU:C     | 2.54                     | 0.45              |
| 9:AI:125:TYR:HD2   | 9:AI:126:SER:H     | 1.64                     | 0.45              |
| 12:AL:119:LYS:O    | 12:AL:120:TYR:CB   | 2.64                     | 0.45              |
| 13:AM:19:LEU:HD22  | 13:AM:19:LEU:N     | 2.31                     | 0.45              |
| 13:AM:4:ILE:CG2    | 13:AM:5:ALA:H      | 2.23                     | 0.45              |
| 13:AM:54:VAL:HG12  | 13:AM:58:GLU:CG    | 2.46                     | 0.45              |
| 17:AQ:88:TYR:O     | 17:AQ:91:ARG:N     | 2.50                     | 0.45              |
| 19:AS:72:GLY:C     | 19:AS:74:PHE:N     | 2.70                     | 0.45              |
| 20:AT:50:GLU:HG3   | 20:AT:51:GLU:H     | 1.78                     | 0.45              |
| 22:AV:38:A:H2'     | 22:AV:39:C:O4'     | 2.16                     | 0.45              |
| 24:AY:15:ILE:C     | 24:AY:101:LEU:HD13 | 2.37                     | 0.45              |
| 24:AY:408:VAL:HG22 | 24:AY:454:MET:HA   | 1.98                     | 0.45              |
| 24:AY:498:ILE:HG22 | 24:AY:507:TYR:CG   | 2.51                     | 0.45              |
| 24:AY:545:GLY:CA   | 24:AY:583:LYS:HG2  | 2.46                     | 0.45              |
| 24:AY:88:VAL:O     | 24:AY:90:PHE:N     | 2.49                     | 0.45              |
| 31:B6:33:LYS:HG2   | 31:B6:34:LEU:H     | 1.81                     | 0.45              |
| 34:B9:34:GLN:O     | 34:B9:35:ARG:CB    | 2.64                     | 0.45              |
| 35:BA:1058:G:N2    | 44:BK:126:MET:HE3  | 2.31                     | 0.45              |
| 35:BA:1237:A:O2'   | 35:BA:1238:G:P     | 2.74                     | 0.45              |
| 35:BA:1385:G:H4'   | 35:BA:1386:C:OP1   | 2.17                     | 0.45              |
| 35:BA:2131:G:C8    | 35:BA:2133:G:N3    | 2.84                     | 0.45              |
| 35:BA:2208:A:H1'   | 35:BA:2219:G:C4    | 2.50                     | 0.45              |
| 35:BA:2466:C:C2'   | 35:BA:2467:C:H5'   | 2.46                     | 0.45              |
| 35:BA:2514:U:C2    | 35:BA:2515:C:C5    | 3.04                     | 0.45              |
| 35:BA:2001:A:H4'   | 35:BA:2689:U:H2'   | 1.99                     | 0.45              |
| 35:BA:272(G):C:H42 | 35:BA:363(C):G:H1  | 1.63                     | 0.45              |
| 35:BA:2742:C:HO2'  | 35:BA:2743:C:H5'   | 1.79                     | 0.45              |
| 35:BA:2787:C:O2    | 35:BA:2787:C:H2'   | 2.17                     | 0.45              |
| 35:BA:753:C:H2'    | 35:BA:754:C:C6     | 2.51                     | 0.45              |
| 35:BA:786:C:C2'    | 35:BA:787:U:H5'    | 2.46                     | 0.45              |
| 35:BA:814:C:N3     | 35:BA:1193:G:O6    | 2.49                     | 0.45              |
| 35:BA:85:G:N3      | 35:BA:103:A:C2     | 2.84                     | 0.45              |
| 37:BC:76:LEU:HB3   | 37:BC:114:VAL:HA   | 1.99                     | 0.45              |
| 38:BD:70:TRP:CD1   | 38:BD:70:TRP:C     | 2.89                     | 0.45              |
| 39:BE:23:VAL:CG1   | 39:BE:173:VAL:HG21 | 2.46                     | 0.45              |
| 39:BE:9:VAL:HG13   | 39:BE:25:VAL:O     | 2.15                     | 0.45              |
| 41:BG:77:ILE:HG22  | 41:BG:80:PHE:CA    | 2.42                     | 0.45              |
| 42:BH:121:ILE:HA   | 42:BH:134:SER:O    | 2.16                     | 0.45              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:BH:146:ALA:O    | 42:BH:147:ASN:C    | 2.55                     | 0.45              |
| 44:BK:105:LEU:CD2  | 44:BK:120:LEU:HD13 | 2.46                     | 0.45              |
| 48:BP:99:LEU:HG    | 48:BP:100:LEU:HD22 | 1.97                     | 0.45              |
| 48:BP:95:VAL:CG2   | 48:BP:125:VAL:HG23 | 2.44                     | 0.45              |
| 33:B8:59:LYS:HD3   | 48:BP:50:ARG:HB3   | 1.99                     | 0.45              |
| 30:B5:44:THR:CG2   | 50:BR:101:ALA:HB2  | 2.30                     | 0.45              |
| 35:BA:2850:A:C2    | 50:BR:61:HIS:CD2   | 3.03                     | 0.45              |
| 52:BT:102:ILE:O    | 52:BT:103:ARG:C    | 2.55                     | 0.45              |
| 52:BT:29:ARG:HD2   | 52:BT:29:ARG:HA    | 1.72                     | 0.45              |
| 56:BX:41:ASN:HA    | 56:BX:44:GLU:HG2   | 1.97                     | 0.45              |
| 1:CA:1198:G:C6     | 1:CA:1199:U:N3     | 2.84                     | 0.45              |
| 1:CA:1277:C:C3'    | 1:CA:1277:C:C6     | 3.00                     | 0.45              |
| 1:CA:1511:G:C2'    | 1:CA:1512:U:H5'    | 2.46                     | 0.45              |
| 1:CA:311:C:HO2'    | 1:CA:312:C:H5'     | 1.81                     | 0.45              |
| 1:CA:399:G:H2'     | 1:CA:400:C:C6      | 2.51                     | 0.45              |
| 1:CA:495:A:H4'     | 1:CA:496:A:OP1     | 2.15                     | 0.45              |
| 1:CA:666:G:N2      | 1:CA:667:G:H1'     | 2.32                     | 0.45              |
| 1:CA:923:A:H2'     | 1:CA:924:C:C6      | 2.51                     | 0.45              |
| 2:CB:164:VAL:CG1   | 2:CB:165:VAL:N     | 2.79                     | 0.45              |
| 2:CB:32:ILE:CD1    | 2:CB:40:HIS:HB3    | 2.46                     | 0.45              |
| 2:CB:96:ARG:N      | 2:CB:96:ARG:CD     | 2.79                     | 0.45              |
| 4:CD:168:ARG:HH11  | 4:CD:168:ARG:HA    | 1.80                     | 0.45              |
| 6:CF:67:MET:CE     | 6:CF:72:VAL:HA     | 2.46                     | 0.45              |
| 7:CG:97:GLN:O      | 7:CG:98:SER:C      | 2.53                     | 0.45              |
| 11:CK:107:SER:C    | 11:CK:108:ILE:HD12 | 2.36                     | 0.45              |
| 17:CQ:33:GLY:O     | 17:CQ:34:LYS:C     | 2.55                     | 0.45              |
| 22:CV:20:U:H5'     | 22:CV:21:A:OP2     | 2.16                     | 0.45              |
| 24:CY:148:LEU:CD1  | 24:CY:151:ARG:HH11 | 2.29                     | 0.45              |
| 24:CY:190:ASN:HD21 | 24:CY:195:ASP:HB2  | 1.81                     | 0.45              |
| 24:CY:259:PHE:N    | 24:CY:259:PHE:CD1  | 2.84                     | 0.45              |
| 24:CY:264:LEU:HD22 | 24:CY:265:LYS:NZ   | 2.31                     | 0.45              |
| 24:CY:426:GLN:O    | 24:CY:427:ALA:C    | 2.54                     | 0.45              |
| 24:CY:659:LEU:HD13 | 24:CY:659:LEU:C    | 2.36                     | 0.45              |
| 29:D4:22:ILE:H     | 29:D4:22:ILE:HD12  | 1.81                     | 0.45              |
| 31:D6:11:LEU:HD12  | 31:D6:25:LYS:HA    | 1.99                     | 0.45              |
| 35:DA:1114:G:O2'   | 35:DA:1115:G:H5''  | 2.17                     | 0.45              |
| 35:DA:1132:A:C4    | 35:DA:1133:U:C5    | 3.04                     | 0.45              |
| 35:DA:1345:C:C2'   | 35:DA:1346:G:H5'   | 2.47                     | 0.45              |
| 35:DA:134:C:O2'    | 35:DA:135:G:H5'    | 2.17                     | 0.45              |
| 35:DA:1487:G:H3'   | 35:DA:1488:G:H8    | 1.82                     | 0.45              |
| 35:DA:2011:U:C2'   | 35:DA:2012:G:H5'   | 2.47                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:D6:5:VAL:HB     | 35:DA:2284:C:P     | 2.55                     | 0.45              |
| 35:DA:238:C:H2'    | 35:DA:239:U:O4'    | 2.15                     | 0.45              |
| 35:DA:2642:G:O2'   | 35:DA:2643:G:H5'   | 2.16                     | 0.45              |
| 35:DA:271(C):C:H2' | 35:DA:271(D):G:H8  | 1.81                     | 0.45              |
| 35:DA:2732:G:H5''  | 35:DA:2733:A:C8    | 2.51                     | 0.45              |
| 35:DA:2795:G:N3    | 35:DA:2795:G:H2'   | 2.30                     | 0.45              |
| 35:DA:2850:A:C2    | 50:DR:61:HIS:CD2   | 3.05                     | 0.45              |
| 35:DA:272(G):C:H42 | 35:DA:363(C):G:H1  | 1.64                     | 0.45              |
| 35:DA:759:G:H2'    | 35:DA:760:G:C8     | 2.48                     | 0.45              |
| 36:DB:81:G:C2      | 36:DB:82:G:N7      | 2.84                     | 0.45              |
| 41:DG:23:PHE:CE2   | 41:DG:168:GLU:HG2  | 2.51                     | 0.45              |
| 42:DH:89:ILE:O     | 42:DH:89:ILE:CG1   | 2.63                     | 0.45              |
| 44:DK:23:VAL:HG12  | 44:DK:23:VAL:O     | 2.16                     | 0.45              |
| 48:DP:115:LEU:HA   | 48:DP:134:ALA:CB   | 2.42                     | 0.45              |
| 48:DP:98:GLU:HA    | 48:DP:101:VAL:HG22 | 1.98                     | 0.45              |
| 49:DQ:63:LYS:NZ    | 58:DZ:175:VAL:HG21 | 2.30                     | 0.45              |
| 51:DS:13:ARG:O     | 51:DS:14:VAL:HB    | 2.16                     | 0.45              |
| 56:DX:12:VAL:HG12  | 56:DX:27:THR:C     | 2.35                     | 0.45              |
| 57:DY:12:THR:HA    | 57:DY:25:GLY:O     | 2.16                     | 0.45              |
| 58:DZ:44:PHE:C     | 58:DZ:44:PHE:CD1   | 2.88                     | 0.45              |
| 1:AA:1298:C:C5     | 7:AG:114:ARG:HD3   | 2.51                     | 0.45              |
| 1:AA:1351:U:O5'    | 1:AA:1351:U:H6     | 2.00                     | 0.45              |
| 1:AA:1452:C:OP1    | 1:AA:1452:C:O4'    | 2.34                     | 0.45              |
| 1:AA:1515:C:O2'    | 1:AA:1516:G:H5'    | 2.16                     | 0.45              |
| 1:AA:356:A:H2'     | 1:AA:357:G:H8      | 1.81                     | 0.45              |
| 1:AA:56:U:H2'      | 1:AA:57:G:C8       | 2.52                     | 0.45              |
| 1:AA:763:G:H2'     | 1:AA:764:C:H6      | 1.82                     | 0.45              |
| 1:AA:771:G:H2'     | 1:AA:772:U:H6      | 1.82                     | 0.45              |
| 2:AB:169:LYS:HD3   | 2:AB:169:LYS:O     | 2.16                     | 0.45              |
| 2:AB:17:PHE:CG     | 2:AB:18:GLY:N      | 2.85                     | 0.45              |
| 2:AB:207:ALA:O     | 2:AB:208:ILE:C     | 2.55                     | 0.45              |
| 2:AB:8:LYS:O       | 2:AB:9:GLU:C       | 2.54                     | 0.45              |
| 3:AC:83:ARG:C      | 3:AC:85:ARG:H      | 2.20                     | 0.45              |
| 1:AA:542:G:P       | 4:AD:10:ARG:HH21   | 2.39                     | 0.45              |
| 7:AG:88:PRO:HG2    | 7:AG:88:PRO:O      | 2.16                     | 0.45              |
| 8:AH:122:ARG:HB3   | 8:AH:122:ARG:HH11  | 1.82                     | 0.45              |
| 12:AL:42:THR:O     | 12:AL:42:THR:HG23  | 2.16                     | 0.45              |
| 15:AO:74:ASP:O     | 15:AO:76:GLU:N     | 2.49                     | 0.45              |
| 22:AV:59:A:C2'     | 22:AV:60:U:H5'     | 2.47                     | 0.45              |
| 22:AV:72:A:C6      | 22:AV:73:A:C6      | 3.03                     | 0.45              |
| 24:AY:166:LEU:N    | 24:AY:166:LEU:HD12 | 2.31                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:B2:64:LEU:C     | 27:B2:64:LEU:HD13  | 2.37                     | 0.45              |
| 30:B5:7:PRO:HG2    | 35:BA:2016:U:O2    | 2.15                     | 0.45              |
| 35:BA:1146:C:H2'   | 35:BA:1146:C:O2    | 2.16                     | 0.45              |
| 35:BA:1315:C:H42   | 35:BA:1337:G:H1    | 1.65                     | 0.45              |
| 35:BA:1951:U:H2'   | 35:BA:1953:A:OP2   | 2.16                     | 0.45              |
| 30:B5:2:ALA:N      | 35:BA:2015:A:H1'   | 2.30                     | 0.45              |
| 35:BA:2016:U:O2'   | 35:BA:2017:U:H5'   | 2.16                     | 0.45              |
| 34:B9:6:SER:HB2    | 35:BA:2466:C:H5''  | 1.99                     | 0.45              |
| 30:B5:22:HIS:HE1   | 35:BA:2624:G:H1'   | 1.82                     | 0.45              |
| 35:BA:440:G:N2     | 40:BF:46:ARG:NH2   | 2.64                     | 0.45              |
| 35:BA:532:A:N1     | 35:BA:2020:A:H1'   | 2.31                     | 0.45              |
| 35:BA:604:G:O2'    | 35:BA:605:C:H5'    | 2.15                     | 0.45              |
| 25:B0:26:TYR:CE2   | 35:BA:857:C:H1'    | 2.50                     | 0.45              |
| 37:BC:101:ILE:HG13 | 37:BC:128:LEU:CD1  | 2.42                     | 0.45              |
| 35:BA:2202:C:H2'   | 38:BD:151:LYS:HZ3  | 1.80                     | 0.45              |
| 39:BE:36:ARG:NH1   | 39:BE:36:ARG:CG    | 2.75                     | 0.45              |
| 41:BG:55:LYS:HA    | 41:BG:58:GLN:HG3   | 1.98                     | 0.45              |
| 42:BH:173:PRO:HG2  | 42:BH:174:GLY:H    | 1.80                     | 0.45              |
| 44:BK:77:LEU:HD13  | 44:BK:110:GLN:OE1  | 2.15                     | 0.45              |
| 46:BN:120:LEU:C    | 46:BN:120:LEU:HD13 | 2.36                     | 0.45              |
| 46:BN:14:VAL:HG11  | 46:BN:137:LYS:CD   | 2.45                     | 0.45              |
| 47:BO:107:ARG:HA   | 47:BO:112:MET:HE2  | 1.97                     | 0.45              |
| 51:BS:28:VAL:CG1   | 51:BS:29:PHE:H     | 2.13                     | 0.45              |
| 52:BT:118:ARG:HA   | 52:BT:121:ILE:CB   | 2.43                     | 0.45              |
| 52:BT:27:THR:C     | 52:BT:28:VAL:HG23  | 2.34                     | 0.45              |
| 53:BU:13:LYS:O     | 53:BU:16:LYS:HB2   | 2.16                     | 0.45              |
| 53:BU:49:HIS:CA    | 53:BU:52:ARG:HB2   | 2.46                     | 0.45              |
| 35:BA:1155:A:O3'   | 53:BU:55:ARG:NH1   | 2.50                     | 0.45              |
| 54:BV:15:GLU:O     | 54:BV:16:PRO:C     | 2.53                     | 0.45              |
| 57:BY:88:LYS:HE2   | 57:BY:93:GLY:HA3   | 1.99                     | 0.45              |
| 58:BZ:26:GLY:O     | 58:BZ:27:VAL:CB    | 2.64                     | 0.45              |
| 1:CA:1236:A:H2'    | 1:CA:1237:C:C5     | 2.50                     | 0.45              |
| 1:CA:1254:C:H2'    | 1:CA:1255:G:H8     | 1.80                     | 0.45              |
| 1:CA:1291:G:H2'    | 1:CA:1292:U:C6     | 2.51                     | 0.45              |
| 1:CA:1351:U:H6     | 1:CA:1351:U:O5'    | 1.98                     | 0.45              |
| 1:CA:141:A:H1'     | 1:CA:182:U:C2      | 2.50                     | 0.45              |
| 1:CA:542:G:O2'     | 1:CA:543:C:H5'     | 2.16                     | 0.45              |
| 1:CA:743:U:H2'     | 1:CA:744:C:C6      | 2.51                     | 0.45              |
| 1:CA:940:C:O2'     | 1:CA:941:G:H5'     | 2.17                     | 0.45              |
| 2:CB:215:LEU:O     | 2:CB:218:ALA:HB3   | 2.16                     | 0.45              |
| 2:CB:7:VAL:C       | 2:CB:11:LEU:HG     | 2.36                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:CC:53:ALA:HB2    | 3:CC:115:LEU:HG    | 1.97                     | 0.45              |
| 4:CD:127:THR:HG23  | 4:CD:147:ALA:HB3   | 1.99                     | 0.45              |
| 4:CD:13:ARG:O      | 4:CD:16:GLY:N      | 2.39                     | 0.45              |
| 5:CE:136:MET:O     | 5:CE:137:GLU:C     | 2.54                     | 0.45              |
| 5:CE:144:THR:O     | 5:CE:145:LYS:C     | 2.55                     | 0.45              |
| 7:CG:72:ARG:HG3    | 7:CG:73:MET:HG3    | 1.98                     | 0.45              |
| 13:CM:10:PRO:O     | 13:CM:11:ARG:CB    | 2.65                     | 0.45              |
| 3:CC:29:TYR:CG     | 14:CN:36:PHE:HE1   | 2.34                     | 0.45              |
| 15:CO:29:VAL:HG11  | 15:CO:67:LEU:HD21  | 1.99                     | 0.45              |
| 20:CT:26:ASN:N     | 20:CT:26:ASN:HD22  | 2.12                     | 0.45              |
| 21:CU:23:PRO:C     | 21:CU:25:LYS:N     | 2.69                     | 0.45              |
| 22:CV:47:U:OP1     | 22:CV:47:U:H6      | 2.00                     | 0.45              |
| 24:CY:117:GLN:NE2  | 24:CY:120:THR:CG2  | 2.80                     | 0.45              |
| 24:CY:136:ALA:HB3  | 24:CY:260:LEU:CB   | 2.26                     | 0.45              |
| 24:CY:327:PHE:CD2  | 24:CY:376:ALA:HB2  | 2.50                     | 0.45              |
| 24:CY:341:VAL:HG21 | 24:CY:389:LEU:HD23 | 1.98                     | 0.45              |
| 30:D5:11:THR:OG1   | 35:DA:1263:U:O3'   | 2.34                     | 0.45              |
| 35:DA:1080:C:H4'   | 44:DK:125:ARG:CB   | 2.41                     | 0.45              |
| 35:DA:1436:G:H1'   | 35:DA:1477:A:O2'   | 2.15                     | 0.45              |
| 35:DA:1539:G:N3    | 35:DA:1540:U:H1'   | 2.30                     | 0.45              |
| 35:DA:1628:G:O2'   | 35:DA:1629:U:H5'   | 2.17                     | 0.45              |
| 35:DA:2393:A:O2'   | 35:DA:2394:C:H5'   | 2.16                     | 0.45              |
| 35:DA:1638:C:H1'   | 35:DA:2698:U:O2'   | 2.16                     | 0.45              |
| 35:DA:272(H):C:H5' | 35:DA:272(H):C:C6  | 2.33                     | 0.45              |
| 35:DA:657:U:C2     | 35:DA:658:C:C5     | 3.05                     | 0.45              |
| 35:DA:768:G:H2'    | 35:DA:769:G:C8     | 2.52                     | 0.45              |
| 35:DA:904:C:H2'    | 35:DA:905:U:C6     | 2.51                     | 0.45              |
| 36:DB:14:U:H5'     | 36:DB:71:C:O4'     | 2.16                     | 0.45              |
| 37:DC:182:PRO:HB3  | 37:DC:184:GLU:OE2  | 2.16                     | 0.45              |
| 39:DE:32:PRO:CA    | 39:DE:90:THR:HG23  | 2.46                     | 0.45              |
| 39:DE:38:THR:CG2   | 39:DE:40:GLU:HB2   | 2.45                     | 0.45              |
| 39:DE:87:GLU:O     | 39:DE:88:GLY:C     | 2.55                     | 0.45              |
| 40:DF:132:VAL:CG2  | 40:DF:133:ASN:H    | 2.28                     | 0.45              |
| 40:DF:180:GLY:O    | 40:DF:182:ASN:N    | 2.49                     | 0.45              |
| 41:DG:125:PHE:CZ   | 41:DG:173:LEU:HD12 | 2.51                     | 0.45              |
| 41:DG:33:ARG:N     | 41:DG:33:ARG:HD3   | 2.30                     | 0.45              |
| 43:DJ:9:UNK:O      | 43:DJ:11:UNK:N     | 2.48                     | 0.45              |
| 46:DN:67:LEU:HB3   | 46:DN:88:GLU:HG2   | 1.95                     | 0.45              |
| 48:DP:59:LEU:O     | 48:DP:59:LEU:HD23  | 2.17                     | 0.45              |
| 50:DR:92:GLY:HA2   | 50:DR:94:TYR:CE1   | 2.51                     | 0.45              |
| 51:DS:89:ARG:HE    | 51:DS:91:PRO:HG2   | 1.80                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 52:DT:7:ILE:O     | 52:DT:10:VAL:HB   | 2.17                     | 0.45              |
| 53:DU:49:HIS:CA   | 53:DU:52:ARG:HB2  | 2.46                     | 0.45              |
| 53:DU:76:TYR:CE2  | 53:DU:80:ILE:HG13 | 2.51                     | 0.45              |
| 49:DQ:55:VAL:CG2  | 58:DZ:178:GLU:HG3 | 2.46                     | 0.45              |
| 1:AA:1082:G:C2'   | 1:AA:1083:U:H5'   | 2.46                     | 0.45              |
| 1:AA:1504:G:OP1   | 1:AA:1507:A:H4'   | 2.16                     | 0.45              |
| 1:AA:221:C:H5'    | 1:AA:222:U:OP2    | 2.17                     | 0.45              |
| 1:AA:253:U:H2'    | 1:AA:254:G:C8     | 2.51                     | 0.45              |
| 1:AA:472:A:H2'    | 1:AA:473:G:O4'    | 2.16                     | 0.45              |
| 1:AA:943:U:O2'    | 1:AA:944:G:H5'    | 2.17                     | 0.45              |
| 3:AC:187:ALA:C    | 3:AC:188:LEU:HD22 | 2.37                     | 0.45              |
| 3:AC:43:LEU:O     | 3:AC:45:LYS:N     | 2.50                     | 0.45              |
| 5:AE:11:ILE:HG22  | 5:AE:12:LEU:N     | 2.31                     | 0.45              |
| 11:AK:34:ASP:OD2  | 11:AK:34:ASP:C    | 2.55                     | 0.45              |
| 11:AK:38:ASN:HA   | 11:AK:39:PRO:HD3  | 1.83                     | 0.45              |
| 13:AM:106:ASN:O   | 13:AM:107:ALA:CB  | 2.64                     | 0.45              |
| 19:AS:41:VAL:C    | 19:AS:43:GLU:N    | 2.68                     | 0.45              |
| 19:AS:79:THR:CG2  | 19:AS:80:TYR:N    | 2.80                     | 0.45              |
| 22:AV:38:A:O2'    | 22:AV:39:C:H5'    | 2.16                     | 0.45              |
| 24:AY:539:ILE:HA  | 24:AY:542:VAL:CG1 | 2.44                     | 0.45              |
| 26:B1:60:PHE:CE1  | 26:B1:91:LYS:HG3  | 2.51                     | 0.45              |
| 26:B1:68:PRO:C    | 26:B1:70:VAL:N    | 2.70                     | 0.45              |
| 27:B2:35:LEU:HD23 | 27:B2:35:LEU:C    | 2.37                     | 0.45              |
| 28:B3:56:VAL:CG1  | 28:B3:57:GLU:H    | 2.22                     | 0.45              |
| 29:B4:48:ARG:O    | 29:B4:49:PHE:HD1  | 1.99                     | 0.45              |
| 30:B5:56:LYS:CG   | 30:B5:57:VAL:H    | 2.05                     | 0.45              |
| 31:B6:43:CYS:O    | 31:B6:44:ARG:CB   | 2.63                     | 0.45              |
| 35:BA:1058:G:H21  | 44:BK:126:MET:HE1 | 1.82                     | 0.45              |
| 35:BA:1341:U:H4'  | 56:BX:57:LEU:HB3  | 1.99                     | 0.45              |
| 35:BA:1544:A:O2'  | 35:BA:1545:A:H5'  | 2.16                     | 0.45              |
| 35:BA:1635:G:H2'  | 35:BA:1636:C:C6   | 2.50                     | 0.45              |
| 35:BA:1709:U:H3   | 35:BA:1749:A:H61  | 1.65                     | 0.45              |
| 35:BA:1780:A:H5'  | 35:BA:1781:C:OP2  | 2.16                     | 0.45              |
| 35:BA:2037:G:C6   | 35:BA:2038:G:C6   | 3.04                     | 0.45              |
| 35:BA:2134:A:N3   | 35:BA:2134:A:H2'  | 2.31                     | 0.45              |
| 35:BA:2260:C:H2'  | 35:BA:2261:C:C6   | 2.49                     | 0.45              |
| 35:BA:2373:G:H2'  | 35:BA:2374:C:H6   | 1.81                     | 0.45              |
| 35:BA:2443:C:O2   | 35:BA:2443:C:C2'  | 2.65                     | 0.45              |
| 35:BA:2616:C:H2'  | 35:BA:2616:C:O2   | 2.17                     | 0.45              |
| 35:BA:2820:A:C8   | 39:BE:191:PRO:CB  | 2.99                     | 0.45              |
| 35:BA:2836:U:H2'  | 35:BA:2837:G:C8   | 2.51                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:325:G:H2'    | 35:BA:326:G:C8     | 2.52                     | 0.45              |
| 35:BA:42:G:H2'     | 35:BA:42:G:N3      | 2.31                     | 0.45              |
| 37:BC:101:ILE:H    | 37:BC:101:ILE:CD1  | 2.29                     | 0.45              |
| 39:BE:38:THR:C     | 39:BE:40:GLU:H     | 2.20                     | 0.45              |
| 40:BF:29:ASN:O     | 40:BF:30:PRO:C     | 2.55                     | 0.45              |
| 41:BG:81:LYS:O     | 41:BG:83:ARG:HG3   | 2.16                     | 0.45              |
| 24:AY:662:LYS:HZ2  | 42:BH:175:LYS:HG3  | 1.76                     | 0.45              |
| 46:BN:119:ARG:HH11 | 46:BN:119:ARG:HG3  | 1.81                     | 0.45              |
| 47:BO:53:LYS:O     | 47:BO:54:GLU:C     | 2.54                     | 0.45              |
| 40:BF:34:TRP:CB    | 48:BP:10:PRO:HB2   | 2.34                     | 0.45              |
| 49:BQ:52:VAL:O     | 49:BQ:54:MET:N     | 2.50                     | 0.45              |
| 51:BS:97:ARG:O     | 51:BS:97:ARG:NE    | 2.49                     | 0.45              |
| 52:BT:134:GLU:O    | 52:BT:135:ALA:CB   | 2.63                     | 0.45              |
| 53:BU:57:PHE:O     | 53:BU:58:ARG:C     | 2.55                     | 0.45              |
| 1:CA:1408:A:H2'    | 1:CA:1409:C:H6     | 1.81                     | 0.45              |
| 1:CA:1442:G:H8     | 1:CA:1442:G:H3'    | 1.81                     | 0.45              |
| 1:CA:1499:A:H1'    | 1:CA:1520:G:H5'    | 1.99                     | 0.45              |
| 1:CA:243:A:C2      | 1:CA:246:A:C8      | 3.05                     | 0.45              |
| 1:CA:451:A:O4'     | 1:CA:452:A:C8      | 2.69                     | 0.45              |
| 1:CA:533:A:OP1     | 1:CA:533:A:H3'     | 2.17                     | 0.45              |
| 4:CD:163:GLU:C     | 4:CD:165:MET:H     | 2.20                     | 0.45              |
| 7:CG:116:ALA:O     | 7:CG:120:ILE:HG12  | 2.15                     | 0.45              |
| 7:CG:92:SER:O      | 7:CG:93:PRO:C      | 2.54                     | 0.45              |
| 8:CH:19:VAL:HG21   | 8:CH:21:LYS:HE2    | 1.97                     | 0.45              |
| 10:CJ:50:ILE:CD1   | 10:CJ:50:ILE:H     | 2.15                     | 0.45              |
| 13:CM:49:THR:C     | 13:CM:51:ALA:N     | 2.70                     | 0.45              |
| 13:CM:63:THR:CG2   | 13:CM:64:TRP:N     | 2.77                     | 0.45              |
| 16:CP:74:LEU:HD22  | 16:CP:79:VAL:HG21  | 1.98                     | 0.45              |
| 20:CT:69:GLY:O     | 20:CT:73:HIS:NE2   | 2.49                     | 0.45              |
| 20:CT:89:ARG:HD2   | 20:CT:104:LEU:HD11 | 1.98                     | 0.45              |
| 21:CU:18:TYR:CD2   | 21:CU:24:ARG:HA    | 2.51                     | 0.45              |
| 22:CW:8:U:H3       | 22:CW:14:A:N6      | 2.15                     | 0.45              |
| 24:CY:38:ARG:O     | 24:CY:39:ILE:C     | 2.54                     | 0.45              |
| 24:CY:69:VAL:O     | 24:CY:69:VAL:HG13  | 2.17                     | 0.45              |
| 27:D2:41:ILE:O     | 27:D2:41:ILE:HG13  | 2.17                     | 0.45              |
| 30:D5:51:TYR:HD2   | 30:D5:52:TYR:H     | 1.63                     | 0.45              |
| 31:D6:16:CYS:O     | 31:D6:17:LYS:C     | 2.53                     | 0.45              |
| 33:D8:53:PRO:HG2   | 33:D8:54:GLU:H     | 1.82                     | 0.45              |
| 35:DA:85:G:N3      | 35:DA:103:A:C2     | 2.84                     | 0.45              |
| 35:DA:1166:C:H2'   | 35:DA:1167:U:C6    | 2.52                     | 0.45              |
| 35:DA:1209:G:H21   | 35:DA:1210:A:H62   | 1.63                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:DA:1313:U:C2   | 35:DA:1610:A:H2    | 2.35                     | 0.45              |
| 35:DA:182:A:O2'   | 35:DA:183:C:H5'    | 2.17                     | 0.45              |
| 35:DA:2081:C:H2'  | 35:DA:2082:A:H8    | 1.80                     | 0.45              |
| 35:DA:198:C:N4    | 35:DA:248:G:H1     | 2.14                     | 0.45              |
| 35:DA:2551:C:H2'  | 35:DA:2552:U:C6    | 2.51                     | 0.45              |
| 35:DA:291:C:H2'   | 35:DA:292:C:C6     | 2.51                     | 0.45              |
| 35:DA:333:G:H2'   | 35:DA:333:G:N3     | 2.31                     | 0.45              |
| 35:DA:389:G:O4'   | 35:DA:2413:G:C4'   | 2.64                     | 0.45              |
| 35:DA:428:A:H3'   | 35:DA:429:A:H8     | 1.80                     | 0.45              |
| 35:DA:71:A:N3     | 35:DA:73:A:N6      | 2.65                     | 0.45              |
| 35:DA:87:C:OP2    | 35:DA:90:U:O4      | 2.34                     | 0.45              |
| 37:DC:173:HIS:O   | 37:DC:174:ALA:HB2  | 2.17                     | 0.45              |
| 38:DD:24:ILE:CD1  | 38:DD:25:THR:N     | 2.79                     | 0.45              |
| 41:DG:44:GLY:O    | 41:DG:47:LYS:HD3   | 2.16                     | 0.45              |
| 43:DJ:100:UNK:HA  | 43:DJ:103:UNK:CB   | 2.47                     | 0.45              |
| 46:DN:95:PRO:HA   | 46:DN:98:VAL:CG2   | 2.47                     | 0.45              |
| 48:DP:127:ALA:C   | 48:DP:148:LEU:HD11 | 2.37                     | 0.45              |
| 50:DR:96:ARG:O    | 50:DR:114:VAL:HA   | 2.16                     | 0.45              |
| 51:DS:73:LEU:HD23 | 51:DS:73:LEU:O     | 2.16                     | 0.45              |
| 52:DT:82:LEU:CD1  | 52:DT:82:LEU:N     | 2.79                     | 0.45              |
| 53:DU:66:ASN:O    | 53:DU:68:ALA:N     | 2.49                     | 0.45              |
| 58:DZ:145:GLU:OE1 | 58:DZ:146:ILE:HG23 | 2.17                     | 0.45              |
| 35:DA:904:C:O2'   | 58:DZ:169:GLU:OE2  | 2.31                     | 0.45              |
| 1:AA:1123:A:H61   | 1:AA:1149:C:N4     | 2.14                     | 0.45              |
| 1:AA:260:G:H2'    | 1:AA:261:U:C6      | 2.50                     | 0.45              |
| 1:AA:308:C:H2'    | 1:AA:309:G:C8      | 2.51                     | 0.45              |
| 1:AA:32:A:H2'     | 1:AA:33:A:C8       | 2.52                     | 0.45              |
| 2:AB:9:GLU:HG2    | 2:AB:10:LEU:N      | 2.32                     | 0.45              |
| 2:AB:209:ARG:HH11 | 2:AB:239:VAL:HG11  | 1.81                     | 0.45              |
| 3:AC:25:GLY:C     | 3:AC:27:LYS:N      | 2.70                     | 0.45              |
| 3:AC:3:ASN:O      | 3:AC:4:LYS:CB      | 2.60                     | 0.45              |
| 4:AD:125:HIS:C    | 4:AD:126:ILE:HD12  | 2.36                     | 0.45              |
| 4:AD:191:ARG:O    | 4:AD:191:ARG:NH1   | 2.49                     | 0.45              |
| 6:AF:53:ALA:C     | 6:AF:55:ASP:H      | 2.19                     | 0.45              |
| 10:AJ:50:ILE:CD1  | 10:AJ:50:ILE:H     | 2.15                     | 0.45              |
| 11:AK:58:PRO:O    | 11:AK:59:TYR:C     | 2.54                     | 0.45              |
| 12:AL:47:LYS:HZ3  | 12:AL:48:PRO:HD3   | 1.81                     | 0.45              |
| 12:AL:7:ILE:CG2   | 12:AL:8:ASN:N      | 2.80                     | 0.45              |
| 17:AQ:99:SER:O    | 17:AQ:100:LYS:HG3  | 2.17                     | 0.45              |
| 22:AV:9:G:O2'     | 22:AV:10:G:N7      | 2.45                     | 0.45              |
| 22:AW:68:C:H2'    | 22:AW:69:C:C6      | 2.51                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:AY:203:GLU:HA   | 24:AY:203:GLU:OE2  | 2.16                     | 0.45              |
| 24:AY:181:LEU:CD1  | 24:AY:242:LEU:HD22 | 2.46                     | 0.45              |
| 24:AY:334:THR:HG23 | 24:AY:370:LYS:HA   | 1.99                     | 0.45              |
| 24:AY:417:THR:C    | 24:AY:419:ALA:N    | 2.70                     | 0.45              |
| 24:AY:468:ARG:CG   | 24:AY:468:ARG:HH11 | 2.30                     | 0.45              |
| 24:AY:562:ASP:O    | 24:AY:563:ILE:HG23 | 2.15                     | 0.45              |
| 26:B1:4:VAL:HA     | 26:B1:10:LYS:O     | 2.17                     | 0.45              |
| 26:B1:44:PRO:HB2   | 26:B1:46:LEU:HD12  | 1.98                     | 0.45              |
| 27:B2:69:ARG:O     | 27:B2:70:GLN:HB2   | 2.16                     | 0.45              |
| 35:BA:1053:C:H2'   | 35:BA:1054:A:C5'   | 2.42                     | 0.45              |
| 35:BA:1186:G:H2'   | 35:BA:1187:G:H5'   | 1.99                     | 0.45              |
| 35:BA:1331:A:C2'   | 35:BA:1332:G:H5''  | 2.46                     | 0.45              |
| 35:BA:1590:U:H2'   | 35:BA:1591:G:H8    | 1.82                     | 0.45              |
| 35:BA:176:G:C2'    | 35:BA:177:G:H5'    | 2.47                     | 0.45              |
| 35:BA:1782:C:C2'   | 35:BA:1783:A:H5'   | 2.47                     | 0.45              |
| 35:BA:2628:C:O2'   | 35:BA:2781:A:H2'   | 2.17                     | 0.45              |
| 35:BA:718:A:H3'    | 35:BA:719:C:H6     | 1.81                     | 0.45              |
| 37:BC:79:ALA:HB1   | 37:BC:83:LYS:HB2   | 1.97                     | 0.45              |
| 39:BE:32:PRO:HA    | 39:BE:90:THR:HG23  | 1.97                     | 0.45              |
| 35:BA:2784:C:H1'   | 39:BE:37:ARG:NH1   | 2.32                     | 0.45              |
| 35:BA:2787:C:H1'   | 39:BE:61:ARG:HD3   | 1.99                     | 0.45              |
| 40:BF:10:PRO:HD2   | 40:BF:13:SER:O     | 2.16                     | 0.45              |
| 40:BF:26:ALA:O     | 40:BF:27:GLU:HG3   | 2.17                     | 0.45              |
| 40:BF:68:LYS:HG3   | 40:BF:69:HIS:HD2   | 1.81                     | 0.45              |
| 41:BG:91:ARG:CD    | 41:BG:92:VAL:N     | 2.72                     | 0.45              |
| 43:BJ:73:UNK:O     | 43:BJ:74:UNK:C     | 2.63                     | 0.45              |
| 44:BK:23:VAL:HG12  | 44:BK:23:VAL:O     | 2.16                     | 0.45              |
| 46:BN:26:LEU:C     | 46:BN:26:LEU:CD1   | 2.80                     | 0.45              |
| 48:BP:46:LYS:HG2   | 48:BP:52:GLU:HG2   | 1.99                     | 0.45              |
| 30:B5:44:THR:CG2   | 50:BR:101:ALA:N    | 2.80                     | 0.45              |
| 50:BR:59:ASP:O     | 50:BR:60:LEU:C     | 2.55                     | 0.45              |
| 50:BR:97:VAL:O     | 50:BR:98:LEU:HD23  | 2.16                     | 0.45              |
| 51:BS:70:GLY:CA    | 51:BS:101:LEU:HD23 | 2.46                     | 0.45              |
| 54:BV:19:LYS:HG3   | 54:BV:20:LEU:N     | 2.30                     | 0.45              |
| 57:BY:28:LYS:HD2   | 57:BY:37:VAL:HG11  | 1.99                     | 0.45              |
| 57:BY:49:VAL:HG12  | 57:BY:50:ARG:N     | 2.32                     | 0.45              |
| 58:BZ:162:GLU:O    | 58:BZ:163:LEU:O    | 2.35                     | 0.45              |
| 58:BZ:14:LYS:O     | 58:BZ:16:SER:N     | 2.50                     | 0.45              |
| 1:CA:1226:C:C5     | 13:CM:104:ARG:HB2  | 2.52                     | 0.45              |
| 1:CA:841:U:H3'     | 1:CA:848:C:C5'     | 2.47                     | 0.45              |
| 1:CA:923:A:O2'     | 1:CA:924:C:H5'     | 2.17                     | 0.45              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 2:CB:220:ASP:O     | 2:CB:222:ILE:N      | 2.50                     | 0.45              |
| 3:CC:32:LEU:HB3    | 3:CC:59:ARG:HH22    | 1.81                     | 0.45              |
| 3:CC:35:GLU:OE1    | 3:CC:97:LYS:HE3     | 2.17                     | 0.45              |
| 4:CD:189:PRO:HB2   | 4:CD:194:LEU:CD2    | 2.45                     | 0.45              |
| 5:CE:11:ILE:HD13   | 5:CE:105:VAL:HG13   | 1.98                     | 0.45              |
| 7:CG:134:ALA:O     | 7:CG:137:LYS:N      | 2.45                     | 0.45              |
| 8:CH:30:ARG:CB     | 8:CH:30:ARG:HH11    | 2.30                     | 0.45              |
| 11:CK:125:PHE:HD1  | 11:CK:125:PHE:N     | 2.15                     | 0.45              |
| 17:CQ:22:LEU:HD13  | 17:CQ:41:LYS:HG2    | 1.98                     | 0.45              |
| 19:CS:42:PRO:C     | 19:CS:43:GLU:HG3    | 2.37                     | 0.45              |
| 22:CV:5:G:N2       | 22:CV:69:C:C2       | 2.84                     | 0.45              |
| 24:CY:15:ILE:HB    | 24:CY:104:ALA:HA    | 1.97                     | 0.45              |
| 24:CY:112:GLN:HG3  | 24:CY:115:GLU:CA    | 2.46                     | 0.45              |
| 24:CY:120:THR:O    | 24:CY:124:GLN:CD    | 2.55                     | 0.45              |
| 24:CY:439:ARG:N    | 24:CY:452:SER:HB3   | 2.32                     | 0.45              |
| 24:CY:510:VAL:HG22 | 24:CY:534:ILE:CD1   | 2.46                     | 0.45              |
| 29:D4:1:MET:HG2    | 41:DG:98:ARG:NH2    | 2.32                     | 0.45              |
| 30:D5:34:PRO:HG3   | 35:DA:2885:C:O2'    | 2.16                     | 0.45              |
| 35:DA:1127:A:C2'   | 35:DA:1128:A:H5''   | 2.44                     | 0.45              |
| 35:DA:1434:A:H5'   | 35:DA:1435:G:OP2    | 2.17                     | 0.45              |
| 35:DA:1445(A):C:O2 | 35:DA:1445(A):C:H2' | 2.15                     | 0.45              |
| 35:DA:1511:C:H2'   | 35:DA:1512:U:O4'    | 2.16                     | 0.45              |
| 35:DA:1529:G:C2    | 35:DA:1541:G:N2     | 2.84                     | 0.45              |
| 35:DA:154(A):C:H42 | 35:DA:172:C:N4      | 2.14                     | 0.45              |
| 35:DA:2261:C:O2'   | 35:DA:2262:U:H5'    | 2.17                     | 0.45              |
| 25:D0:14:ARG:NH1   | 35:DA:2279:G:O6     | 2.49                     | 0.45              |
| 35:DA:2287:A:N6    | 35:DA:2344:U:C2     | 2.84                     | 0.45              |
| 35:DA:307:G:H21    | 35:DA:330:A:N6      | 2.14                     | 0.45              |
| 35:DA:425:G:H2'    | 35:DA:426:C:H6      | 1.80                     | 0.45              |
| 35:DA:84:A:N3      | 35:DA:85:G:H1'      | 2.32                     | 0.45              |
| 36:DB:89:G:N1      | 36:DB:90:A:C2       | 2.85                     | 0.45              |
| 39:DE:165:VAL:HB   | 39:DE:189:PRO:HB3   | 1.99                     | 0.45              |
| 40:DF:2:LYS:CD     | 40:DF:25:PRO:HG2    | 2.46                     | 0.45              |
| 36:DB:56:G:H4'     | 41:DG:27:ASN:HD21   | 1.81                     | 0.45              |
| 46:DN:61:ARG:HG3   | 46:DN:61:ARG:HH11   | 1.82                     | 0.45              |
| 48:DP:5:ASP:OD2    | 48:DP:9:ASN:ND2     | 2.50                     | 0.45              |
| 48:DP:71:VAL:HG12  | 48:DP:72:PRO:HD3    | 1.99                     | 0.45              |
| 48:DP:88:LEU:HD11  | 48:DP:95:VAL:HG11   | 1.99                     | 0.45              |
| 49:DQ:12:GLN:NE2   | 49:DQ:72:LYS:HA     | 2.32                     | 0.45              |
| 35:DA:910:A:C6     | 49:DQ:13:GLN:HG3    | 2.51                     | 0.45              |
| 52:DT:50:ILE:HG23  | 52:DT:99:LEU:O      | 2.16                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:DT:96:ARG:CZ    | 52:DT:96:ARG:HB3   | 2.47                     | 0.45              |
| 54:DV:32:THR:HG22  | 54:DV:33:VAL:N     | 2.32                     | 0.45              |
| 54:DV:4:ILE:HA     | 54:DV:12:TYR:O     | 2.17                     | 0.45              |
| 57:DY:105:ALA:O    | 57:DY:106:LEU:HB2  | 2.17                     | 0.45              |
| 1:AA:1009:G:C2     | 1:AA:1010:G:C8     | 3.04                     | 0.45              |
| 1:AA:129(A):G:C6   | 1:AA:189(E):U:H4'  | 2.52                     | 0.45              |
| 1:AA:1329:A:H4'    | 13:AM:24:GLY:O     | 2.16                     | 0.45              |
| 1:AA:1352:C:OP1    | 21:AU:3:LYS:CE     | 2.65                     | 0.45              |
| 1:AA:1363(A):A:C4' | 1:AA:1364:U:H5''   | 2.42                     | 0.45              |
| 1:AA:1402:C:H2'    | 1:AA:1403:C:O4'    | 2.16                     | 0.45              |
| 1:AA:665:A:H2'     | 1:AA:725:G:N2      | 2.31                     | 0.45              |
| 1:AA:836:G:C6      | 1:AA:851:G:C6      | 3.04                     | 0.45              |
| 3:AC:136:GLN:O     | 3:AC:138:VAL:N     | 2.50                     | 0.45              |
| 3:AC:87:LEU:O      | 3:AC:88:ARG:C      | 2.55                     | 0.45              |
| 5:AE:50:GLU:HB3    | 5:AE:53:LEU:HG     | 1.97                     | 0.45              |
| 12:AL:38:THR:HG23  | 12:AL:57:LYS:CB    | 2.46                     | 0.45              |
| 13:AM:106:ASN:HB3  | 13:AM:107:ALA:H    | 1.53                     | 0.45              |
| 1:AA:452:A:H4'     | 16:AP:72:ARG:CZ    | 2.47                     | 0.45              |
| 21:AU:18:TYR:CD2   | 21:AU:24:ARG:HA    | 2.52                     | 0.45              |
| 22:AV:50:U:O2'     | 22:AV:51:C:H5'     | 2.16                     | 0.45              |
| 22:AW:42:C:C2      | 22:AW:43:G:C8      | 3.05                     | 0.45              |
| 24:AY:259:PHE:CE2  | 24:AY:275:ALA:HB2  | 2.51                     | 0.45              |
| 24:AY:334:THR:HG23 | 24:AY:369:LEU:O    | 2.16                     | 0.45              |
| 24:AY:422:GLU:O    | 24:AY:423:LYS:C    | 2.54                     | 0.45              |
| 31:B6:15:GLU:CD    | 31:B6:44:ARG:HH22  | 2.18                     | 0.45              |
| 35:BA:1196:C:O4'   | 35:BA:1226:A:C2    | 2.70                     | 0.45              |
| 35:BA:1434:A:H5'   | 35:BA:1435:G:OP2   | 2.16                     | 0.45              |
| 35:BA:1572:A:O2'   | 35:BA:1573:G:H5'   | 2.17                     | 0.45              |
| 35:BA:1596:A:C2'   | 35:BA:1597:A:H5'   | 2.46                     | 0.45              |
| 35:BA:688:U:H5'    | 35:BA:1780:A:H2    | 1.82                     | 0.45              |
| 35:BA:2011:U:C2'   | 35:BA:2012:G:H5'   | 2.46                     | 0.45              |
| 35:BA:2131:G:C8    | 35:BA:2133:G:N2    | 2.85                     | 0.45              |
| 35:BA:214:G:H2'    | 35:BA:215:G:O4'    | 2.16                     | 0.45              |
| 35:BA:2521:C:O2    | 35:BA:2521:C:H2'   | 2.15                     | 0.45              |
| 35:BA:271(K):U:H3' | 35:BA:271(L):U:C5' | 2.47                     | 0.45              |
| 35:BA:2840:C:H5''  | 50:BR:53:HIS:CD2   | 2.52                     | 0.45              |
| 35:BA:602:G:N1     | 35:BA:654(U):A:N7  | 2.65                     | 0.45              |
| 35:BA:603:A:O2'    | 35:BA:604:G:P      | 2.75                     | 0.45              |
| 36:BB:40:U:H5''    | 36:BB:41:U:OP2     | 2.16                     | 0.45              |
| 37:BC:191:ARG:NH1  | 37:BC:191:ARG:HG3  | 2.31                     | 0.45              |
| 38:BD:197:GLY:O    | 38:BD:198:ASN:HB3  | 2.17                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:BE:145:LYS:O    | 39:BE:146:THR:C    | 2.54                     | 0.45              |
| 39:BE:27:LEU:HD12  | 39:BE:181:LEU:HD13 | 1.99                     | 0.45              |
| 39:BE:67:PHE:O     | 39:BE:70:ALA:HB2   | 2.17                     | 0.45              |
| 39:BE:68:ALA:O     | 39:BE:70:ALA:N     | 2.49                     | 0.45              |
| 39:BE:2:LYS:CD     | 39:BE:95:ILE:HG22  | 2.47                     | 0.45              |
| 40:BF:112:MET:HA   | 40:BF:115:ALA:HB3  | 1.99                     | 0.45              |
| 40:BF:2:LYS:CD     | 40:BF:25:PRO:HG2   | 2.47                     | 0.45              |
| 41:BG:133:LEU:HD12 | 41:BG:133:LEU:O    | 2.16                     | 0.45              |
| 41:BG:58:GLN:C     | 41:BG:60:LEU:N     | 2.69                     | 0.45              |
| 42:BH:68:THR:C     | 42:BH:70:THR:N     | 2.69                     | 0.45              |
| 42:BH:94:TYR:HA    | 42:BH:106:THR:O    | 2.17                     | 0.45              |
| 44:BK:17:ALA:HB3   | 44:BK:38:VAL:CG1   | 2.47                     | 0.45              |
| 46:BN:135:PRO:O    | 46:BN:136:GLU:C    | 2.55                     | 0.45              |
| 46:BN:96:GLU:O     | 46:BN:100:GLU:HG3  | 2.17                     | 0.45              |
| 48:BP:126:VAL:HG12 | 48:BP:148:LEU:HD21 | 1.99                     | 0.45              |
| 48:BP:25:SER:O     | 48:BP:30:THR:CG2   | 2.65                     | 0.45              |
| 50:BR:12:ARG:CG    | 50:BR:12:ARG:NH1   | 2.78                     | 0.45              |
| 54:BV:35:LEU:HB3   | 54:BV:37:VAL:CG2   | 2.47                     | 0.45              |
| 57:BY:9:LYS:O      | 57:BY:28:LYS:HE2   | 2.17                     | 0.45              |
| 1:CA:1231:G:C2'    | 1:CA:1232:U:H5'    | 2.46                     | 0.45              |
| 1:CA:1234:C:HO2'   | 1:CA:1364:U:H6     | 1.62                     | 0.45              |
| 1:CA:1416:G:O2'    | 1:CA:1417:G:H5'    | 2.17                     | 0.45              |
| 1:CA:403:C:H2'     | 1:CA:404:U:H6      | 1.81                     | 0.45              |
| 1:CA:50:A:N6       | 1:CA:361:G:C4'     | 2.76                     | 0.45              |
| 1:CA:56:U:H2'      | 1:CA:57:G:C8       | 2.52                     | 0.45              |
| 1:CA:57:G:H2'      | 1:CA:58:C:C6       | 2.51                     | 0.45              |
| 1:CA:695:A:H2'     | 1:CA:696:A:C8      | 2.51                     | 0.45              |
| 1:CA:812:C:O2'     | 1:CA:813:U:P       | 2.73                     | 0.45              |
| 2:CB:126:GLU:O     | 2:CB:129:GLU:OE2   | 2.34                     | 0.45              |
| 2:CB:15:VAL:C      | 2:CB:16:HIS:CG     | 2.89                     | 0.45              |
| 2:CB:178:ARG:CG    | 2:CB:178:ARG:HH11  | 2.30                     | 0.45              |
| 3:CC:105:GLU:HG2   | 3:CC:106:VAL:N     | 2.30                     | 0.45              |
| 5:CE:139:LEU:C     | 5:CE:141:GLN:N     | 2.70                     | 0.45              |
| 7:CG:138:LYS:HE3   | 7:CG:142:GLU:OE1   | 2.17                     | 0.45              |
| 9:CI:79:LEU:HD13   | 9:CI:83:ARG:CB     | 2.41                     | 0.45              |
| 10:CJ:22:LYS:HZ2   | 10:CJ:88:LEU:HD23  | 1.81                     | 0.45              |
| 12:CL:38:THR:CG2   | 12:CL:57:LYS:HB3   | 2.46                     | 0.45              |
| 12:CL:33:ARG:HG3   | 12:CL:60:LEU:HD12  | 1.97                     | 0.45              |
| 12:CL:7:ILE:HA     | 12:CL:10:LEU:HD12  | 1.98                     | 0.45              |
| 13:CM:66:LEU:HA    | 13:CM:70:LEU:CD1   | 2.47                     | 0.45              |
| 18:CR:30:ASP:C     | 18:CR:32:ARG:H     | 2.19                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:CR:37:VAL:O     | 18:CR:41:LYS:N     | 2.38                     | 0.45              |
| 11:CK:109:VAL:HG13 | 18:CR:85:LEU:O     | 2.15                     | 0.45              |
| 1:CA:1352:C:OP1    | 21:CU:3:LYS:HE2    | 2.16                     | 0.45              |
| 21:CU:6:ARG:NH2    | 21:CU:15:ARG:HH22  | 2.14                     | 0.45              |
| 24:CY:182:ARG:C    | 24:CY:184:LYS:N    | 2.70                     | 0.45              |
| 24:CY:448:GLN:NE2  | 24:CY:480:GLN:HE21 | 2.14                     | 0.45              |
| 24:CY:592:GLU:HA   | 24:CY:595:GLN:CB   | 2.43                     | 0.45              |
| 24:CY:622:GLY:O    | 35:DA:2473:U:O2    | 2.35                     | 0.45              |
| 61:CY:702:FUA:O2   | 61:CY:702:FUA:H211 | 2.16                     | 0.45              |
| 26:D1:53:VAL:HG22  | 26:D1:74:VAL:HG13  | 1.99                     | 0.45              |
| 26:D1:60:PHE:CE1   | 26:D1:91:LYS:HG3   | 2.52                     | 0.45              |
| 27:D2:32:LEU:CA    | 27:D2:53:LEU:HD13  | 2.38                     | 0.45              |
| 30:D5:58:LEU:C     | 30:D5:58:LEU:HD22  | 2.37                     | 0.45              |
| 31:D6:11:LEU:O     | 31:D6:11:LEU:HD13  | 2.17                     | 0.45              |
| 31:D6:29:ASN:CG    | 31:D6:30:THR:N     | 2.70                     | 0.45              |
| 33:D8:48:PHE:O     | 33:D8:49:VAL:CG2   | 2.62                     | 0.45              |
| 34:D9:29:ASN:O     | 34:D9:31:LYS:N     | 2.49                     | 0.45              |
| 35:DA:1015:G:H2'   | 35:DA:1016:G:C8    | 2.51                     | 0.45              |
| 35:DA:1342:A:O2'   | 35:DA:1344:G:OP2   | 2.30                     | 0.45              |
| 35:DA:1386:C:H5''  | 35:DA:1396:U:H5    | 1.81                     | 0.45              |
| 35:DA:1463:C:H2'   | 35:DA:1464:C:H6    | 1.82                     | 0.45              |
| 35:DA:2163:C:H2'   | 35:DA:2164:C:H5'   | 1.98                     | 0.45              |
| 35:DA:2576:G:N3    | 35:DA:2576:G:H3'   | 2.32                     | 0.45              |
| 35:DA:324:A:N6     | 35:DA:338:G:O2'    | 2.50                     | 0.45              |
| 35:DA:528:A:N1     | 35:DA:2042:A:H2'   | 2.32                     | 0.45              |
| 35:DA:541:C:H42    | 35:DA:552:G:H1     | 1.65                     | 0.45              |
| 37:DC:139:PRO:HA   | 37:DC:145:THR:CB   | 2.47                     | 0.45              |
| 37:DC:86:GLU:O     | 37:DC:90:ALA:HB2   | 2.16                     | 0.45              |
| 38:DD:124:PRO:O    | 38:DD:129:ASN:ND2  | 2.49                     | 0.45              |
| 38:DD:28:GLU:OE1   | 38:DD:29:PRO:HD2   | 2.17                     | 0.45              |
| 40:DF:167:ALA:HA   | 40:DF:170:LEU:HD23 | 1.98                     | 0.45              |
| 41:DG:112:PRO:O    | 41:DG:113:ARG:HG2  | 2.17                     | 0.45              |
| 41:DG:52:ILE:HG22  | 41:DG:53:LEU:N     | 2.32                     | 0.45              |
| 29:D4:9:LEU:HD23   | 41:DG:65:GLY:HA3   | 1.98                     | 0.45              |
| 41:DG:67:LYS:HA    | 41:DG:68:PRO:HD3   | 1.73                     | 0.45              |
| 41:DG:97:ASP:H     | 41:DG:100:TRP:HD1  | 1.65                     | 0.45              |
| 46:DN:55:VAL:HG22  | 46:DN:56:ASN:N     | 2.32                     | 0.45              |
| 51:DS:56:LEU:C     | 51:DS:58:LEU:H     | 2.19                     | 0.45              |
| 51:DS:56:LEU:O     | 51:DS:58:LEU:N     | 2.50                     | 0.45              |
| 53:DU:57:PHE:O     | 53:DU:58:ARG:C     | 2.53                     | 0.45              |
| 1:AA:1103:C:H5''   | 2:AB:98:LEU:HD13   | 1.99                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1226:C:H5''   | 13:AM:103:THR:HB   | 1.97                     | 0.45              |
| 1:AA:1321:C:H3'    | 1:AA:1322:C:C5'    | 2.33                     | 0.45              |
| 1:AA:1506:U:O2'    | 1:AA:1507:A:H5'    | 2.17                     | 0.45              |
| 1:AA:622:A:C8      | 1:AA:623:C:C6      | 3.04                     | 0.45              |
| 1:AA:830:G:H2'     | 1:AA:831:U:H6      | 1.82                     | 0.45              |
| 2:AB:73:THR:HG23   | 2:AB:170:GLU:OE2   | 2.16                     | 0.45              |
| 3:AC:64:VAL:HG12   | 3:AC:66:VAL:HG23   | 1.99                     | 0.45              |
| 4:AD:163:GLU:OE2   | 4:AD:163:GLU:HA    | 2.17                     | 0.45              |
| 9:AI:95:LYS:HZ2    | 9:AI:96:LEU:CD1    | 2.30                     | 0.45              |
| 10:AJ:58:ASP:O     | 10:AJ:59:SER:O     | 2.35                     | 0.45              |
| 1:AA:36:C:H4'      | 12:AL:122:THR:O    | 2.16                     | 0.45              |
| 15:AO:23:GLY:O     | 15:AO:24:SER:O     | 2.35                     | 0.45              |
| 19:AS:11:VAL:O     | 19:AS:11:VAL:HG13  | 2.17                     | 0.45              |
| 19:AS:7:LYS:HA     | 19:AS:7:LYS:HD3    | 1.75                     | 0.45              |
| 22:AV:74:C:H2'     | 22:AV:75:C:H5'     | 1.99                     | 0.45              |
| 24:AY:446:THR:O    | 24:AY:446:THR:HG23 | 2.16                     | 0.45              |
| 24:AY:513:LYS:HB3  | 24:AY:566:THR:HB   | 1.95                     | 0.45              |
| 25:B0:11:ARG:CB    | 25:B0:11:ARG:HH11  | 2.07                     | 0.45              |
| 26:B1:86:SER:CA    | 26:B1:89:GLU:HB2   | 2.47                     | 0.45              |
| 27:B2:63:VAL:HG12  | 27:B2:67:LYS:CG    | 2.47                     | 0.45              |
| 30:B5:3:LYS:HD2    | 30:B5:5:PRO:CD     | 2.42                     | 0.45              |
| 35:BA:1050:A:C4    | 35:BA:1051:G:H1'   | 2.52                     | 0.45              |
| 35:BA:1487:G:H3'   | 35:BA:1488:G:H8    | 1.82                     | 0.45              |
| 35:BA:1718:G:C5'   | 35:BA:1718:G:H8    | 2.28                     | 0.45              |
| 35:BA:1774:C:H6    | 35:BA:1774:C:O5'   | 1.99                     | 0.45              |
| 35:BA:2103:C:H3'   | 35:BA:2104:G:H5''  | 1.99                     | 0.45              |
| 35:BA:2298:A:N6    | 35:BA:2318:G:C8    | 2.81                     | 0.45              |
| 35:BA:2352:A:C2'   | 35:BA:2353:G:H5'   | 2.47                     | 0.45              |
| 35:BA:238:C:H2'    | 35:BA:239:U:O4'    | 2.16                     | 0.45              |
| 35:BA:246:C:C2'    | 35:BA:247:G:H5'    | 2.46                     | 0.45              |
| 35:BA:2642:G:O2'   | 35:BA:2643:G:H5'   | 2.16                     | 0.45              |
| 35:BA:271(Z):C:H1' | 35:BA:272(C):G:H1' | 1.98                     | 0.45              |
| 35:BA:7:G:H1       | 35:BA:2896:C:N4    | 2.15                     | 0.45              |
| 35:BA:311:A:H5'    | 35:BA:332:A:N3     | 2.32                     | 0.45              |
| 38:BD:24:ILE:CD1   | 38:BD:25:THR:N     | 2.78                     | 0.45              |
| 38:BD:270:ILE:HD12 | 38:BD:270:ILE:H    | 1.80                     | 0.45              |
| 39:BE:131:ALA:HB3  | 39:BE:134:ILE:CD1  | 2.17                     | 0.45              |
| 39:BE:69:LYS:HD3   | 39:BE:89:ASP:HA    | 1.98                     | 0.45              |
| 40:BF:118:ALA:O    | 40:BF:121:GLY:N    | 2.49                     | 0.45              |
| 40:BF:132:VAL:CG2  | 40:BF:133:ASN:N    | 2.79                     | 0.45              |
| 41:BG:138:GLN:HG3  | 41:BG:144:ILE:CD1  | 2.46                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:BG:153:ARG:HH11 | 41:BG:153:ARG:CB   | 2.29                     | 0.45              |
| 42:BH:86:GLU:OE2   | 42:BH:86:GLU:N     | 2.49                     | 0.45              |
| 42:BH:94:TYR:CD1   | 42:BH:94:TYR:N     | 2.84                     | 0.45              |
| 43:BJ:26:UNK:HA    | 43:BJ:85:UNK:N     | 2.31                     | 0.45              |
| 49:BQ:12:GLN:NE2   | 49:BQ:72:LYS:HA    | 2.32                     | 0.45              |
| 50:BR:34:ILE:O     | 50:BR:113:LEU:HD12 | 2.17                     | 0.45              |
| 54:BV:1:MET:HB3    | 54:BV:2:PHE:H      | 1.54                     | 0.45              |
| 54:BV:39:LEU:HD12  | 54:BV:47:VAL:HG11  | 1.99                     | 0.45              |
| 55:BW:20:VAL:HG23  | 55:BW:21:VAL:H     | 1.82                     | 0.45              |
| 58:BZ:74:VAL:HG22  | 58:BZ:86:VAL:HG13  | 1.97                     | 0.45              |
| 58:BZ:95:PRO:HA    | 58:BZ:129:SER:HA   | 1.99                     | 0.45              |
| 1:CA:1217:C:O2     | 1:CA:1217:C:H2'    | 2.16                     | 0.45              |
| 1:CA:697:U:H2'     | 1:CA:698:G:C5'     | 2.38                     | 0.45              |
| 1:CA:830:G:H2'     | 1:CA:831:U:H6      | 1.81                     | 0.45              |
| 2:CB:119:GLU:C     | 2:CB:121:LEU:H     | 2.20                     | 0.45              |
| 2:CB:24:TRP:CH2    | 2:CB:26:PRO:HA     | 2.52                     | 0.45              |
| 3:CC:136:GLN:HG3   | 3:CC:139:GLN:CB    | 2.46                     | 0.45              |
| 5:CE:60:TYR:HE1    | 5:CE:64:ARG:NH2    | 2.13                     | 0.45              |
| 9:CI:40:LEU:O      | 9:CI:42:ARG:N      | 2.43                     | 0.45              |
| 13:CM:37:THR:HG21  | 13:CM:56:LEU:CD2   | 2.46                     | 0.45              |
| 13:CM:4:ILE:CG2    | 13:CM:5:ALA:N      | 2.79                     | 0.45              |
| 14:CN:44:LEU:C     | 14:CN:44:LEU:HD12  | 2.37                     | 0.45              |
| 18:CR:40:LEU:C     | 18:CR:42:ARG:N     | 2.67                     | 0.45              |
| 24:CY:282:SER:C    | 24:CY:284:LEU:N    | 2.70                     | 0.45              |
| 24:CY:438:PHE:HD2  | 24:CY:438:PHE:O    | 2.00                     | 0.45              |
| 28:D3:31:LEU:O     | 28:D3:32:GLN:CB    | 2.65                     | 0.45              |
| 29:D4:1:MET:H1     | 36:DB:43:C:H4'     | 1.80                     | 0.45              |
| 31:D6:11:LEU:C     | 31:D6:11:LEU:HD22  | 2.37                     | 0.45              |
| 31:D6:30:THR:O     | 31:D6:31:PRO:C     | 2.55                     | 0.45              |
| 35:DA:1294:U:H6    | 35:DA:1294:U:H5''  | 1.81                     | 0.45              |
| 35:DA:1551:C:H2'   | 35:DA:1552:G:O4'   | 2.16                     | 0.45              |
| 35:DA:1680:U:H2'   | 35:DA:1681:G:O4'   | 2.17                     | 0.45              |
| 35:DA:2305:A:H2'   | 35:DA:2306:C:O4'   | 2.16                     | 0.45              |
| 35:DA:2514:U:C2    | 35:DA:2515:C:C5    | 3.05                     | 0.45              |
| 26:D1:20:ARG:HH12  | 35:DA:387:U:P      | 2.39                     | 0.45              |
| 35:DA:402:A:H2'    | 35:DA:403:U:H5'    | 1.98                     | 0.45              |
| 35:DA:409:C:O2'    | 35:DA:410:G:H5'    | 2.17                     | 0.45              |
| 30:D5:16:ARG:NH2   | 35:DA:517:C:OP1    | 2.49                     | 0.45              |
| 35:DA:531:C:C5     | 35:DA:2035:G:C2    | 3.04                     | 0.45              |
| 35:DA:814:C:N3     | 35:DA:1193:G:O6    | 2.50                     | 0.45              |
| 39:DE:101:ARG:CZ   | 39:DE:171:GLU:HB2  | 2.47                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:DE:132:HIS:HA   | 39:DE:135:HIS:CE1  | 2.51                     | 0.45              |
| 39:DE:177:PRO:HG2  | 39:DE:178:GLU:H    | 1.80                     | 0.45              |
| 39:DE:67:PHE:O     | 39:DE:70:ALA:HB2   | 2.17                     | 0.45              |
| 39:DE:78:LEU:HD12  | 39:DE:78:LEU:O     | 2.16                     | 0.45              |
| 39:DE:93:VAL:C     | 39:DE:95:ILE:H     | 2.20                     | 0.45              |
| 41:DG:114:ILE:HB   | 41:DG:117:PHE:HB2  | 1.98                     | 0.45              |
| 41:DG:98:ARG:N     | 41:DG:98:ARG:HH11  | 2.14                     | 0.45              |
| 42:DH:83:TYR:HA    | 42:DH:135:GLY:O    | 2.16                     | 0.45              |
| 43:DJ:130:UNK:C    | 43:DJ:132:UNK:N    | 2.80                     | 0.45              |
| 44:DK:21:PRO:HA    | 44:DK:23:VAL:H     | 1.81                     | 0.45              |
| 35:DA:558:G:P      | 46:DN:111:PRO:HD2  | 2.56                     | 0.45              |
| 49:DQ:21:THR:O     | 49:DQ:22:LYS:CB    | 2.61                     | 0.45              |
| 52:DT:49:VAL:O     | 52:DT:49:VAL:HG22  | 2.17                     | 0.45              |
| 52:DT:50:ILE:N     | 52:DT:50:ILE:CD1   | 2.78                     | 0.45              |
| 52:DT:83:ILE:CG1   | 52:DT:84:GLN:H     | 2.30                     | 0.45              |
| 54:DV:19:LYS:HG3   | 54:DV:20:LEU:O     | 2.17                     | 0.45              |
| 55:DW:13:SER:HB3   | 55:DW:16:LYS:HD2   | 1.98                     | 0.45              |
| 1:AA:114:U:H2'     | 1:AA:115:G:C8      | 2.52                     | 0.45              |
| 1:AA:1413:A:H2'    | 1:AA:1414:U:O4'    | 2.17                     | 0.45              |
| 1:AA:1522:U:H6     | 1:AA:1522:U:O5'    | 2.00                     | 0.45              |
| 1:AA:193:C:C2      | 1:AA:194:C:C5      | 3.05                     | 0.45              |
| 1:AA:355:C:C4      | 1:AA:356:A:N7      | 2.85                     | 0.45              |
| 1:AA:519:C:H2'     | 1:AA:520:A:O4'     | 2.16                     | 0.45              |
| 1:AA:57:G:H2'      | 1:AA:58:C:C6       | 2.52                     | 0.45              |
| 1:AA:646:U:H2'     | 1:AA:647:C:C6      | 2.52                     | 0.45              |
| 4:AD:25:ARG:O      | 4:AD:28:SER:N      | 2.50                     | 0.45              |
| 4:AD:58:LEU:HD22   | 4:AD:59:ARG:NH1    | 2.32                     | 0.45              |
| 5:AE:101:ILE:CD1   | 5:AE:118:ILE:O     | 2.62                     | 0.45              |
| 5:AE:101:ILE:HD11  | 5:AE:119:LEU:CA    | 2.28                     | 0.45              |
| 5:AE:12:LEU:H      | 5:AE:12:LEU:HD12   | 1.82                     | 0.45              |
| 7:AG:80:VAL:CG2    | 7:AG:81:GLY:H      | 2.27                     | 0.45              |
| 15:AO:43:LEU:CD1   | 15:AO:56:LEU:HD22  | 2.46                     | 0.45              |
| 20:AT:42:GLN:NE2   | 20:AT:42:GLN:CA    | 2.80                     | 0.45              |
| 21:AU:23:PRO:C     | 21:AU:25:LYS:N     | 2.70                     | 0.45              |
| 24:AY:121:VAL:HA   | 24:AY:124:GLN:NE2  | 2.31                     | 0.45              |
| 24:AY:130:VAL:HA   | 24:AY:131:PRO:HD3  | 1.75                     | 0.45              |
| 24:AY:237:PRO:HB2  | 24:AY:242:LEU:HG   | 1.97                     | 0.45              |
| 24:AY:368:GLU:C    | 24:AY:369:LEU:HD12 | 2.36                     | 0.45              |
| 24:AY:519:ARG:HH12 | 24:AY:678:GLU:HB3  | 1.82                     | 0.45              |
| 27:B2:3:LEU:O      | 27:B2:7:ARG:NH1    | 2.49                     | 0.45              |
| 31:B6:30:THR:O     | 31:B6:31:PRO:C     | 2.55                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:B8:50:LEU:C     | 33:B8:52:LYS:H     | 2.17                     | 0.45              |
| 35:BA:2020:A:C6    | 35:BA:2022:U:N3    | 2.84                     | 0.45              |
| 35:BA:2147:G:H2'   | 35:BA:2148:G:C5'   | 2.47                     | 0.45              |
| 35:BA:291:C:H2'    | 35:BA:292:C:C6     | 2.51                     | 0.45              |
| 35:BA:402:A:H2'    | 35:BA:403:U:H5'    | 1.97                     | 0.45              |
| 30:B5:3:LYS:HG2    | 35:BA:747:U:C4     | 2.52                     | 0.45              |
| 36:BB:74:U:O2      | 58:BZ:34:ASN:ND2   | 2.50                     | 0.45              |
| 37:BC:74:ARG:N     | 37:BC:112:ASP:HB2  | 2.29                     | 0.45              |
| 38:BD:144:ALA:HB3  | 38:BD:192:THR:CG2  | 2.43                     | 0.45              |
| 38:BD:67:PHE:CE1   | 38:BD:157:ARG:NH2  | 2.85                     | 0.45              |
| 38:BD:196:VAL:HG12 | 38:BD:196:VAL:O    | 2.16                     | 0.45              |
| 38:BD:39:LYS:HB2   | 38:BD:62:TYR:HB2   | 1.98                     | 0.45              |
| 41:BG:40:ASN:HD22  | 41:BG:91:ARG:HB2   | 1.81                     | 0.45              |
| 42:BH:149:ARG:HA   | 42:BH:162:ILE:CG1  | 2.47                     | 0.45              |
| 47:BO:14:THR:O     | 47:BO:14:THR:HG22  | 2.17                     | 0.45              |
| 47:BO:64:ARG:NH1   | 47:BO:83:ALA:CB    | 2.80                     | 0.45              |
| 48:BP:83:VAL:CG1   | 48:BP:114:ILE:HA   | 2.46                     | 0.45              |
| 48:BP:115:LEU:CD2  | 48:BP:115:LEU:N    | 2.80                     | 0.45              |
| 48:BP:121:LYS:O    | 48:BP:123:LEU:HD23 | 2.16                     | 0.45              |
| 48:BP:95:VAL:HA    | 48:BP:99:LEU:CD2   | 2.41                     | 0.45              |
| 49:BQ:109:VAL:CG1  | 49:BQ:113:GLN:HB2  | 2.47                     | 0.45              |
| 50:BR:65:LEU:O     | 50:BR:65:LEU:HD12  | 2.16                     | 0.45              |
| 51:BS:13:ARG:O     | 51:BS:14:VAL:HB    | 2.17                     | 0.45              |
| 52:BT:14:TYR:CD1   | 52:BT:14:TYR:N     | 2.85                     | 0.45              |
| 53:BU:64:ARG:O     | 53:BU:65:ILE:C     | 2.55                     | 0.45              |
| 54:BV:19:LYS:HG3   | 54:BV:20:LEU:O     | 2.17                     | 0.45              |
| 57:BY:14:LEU:HD13  | 57:BY:24:VAL:CG2   | 2.46                     | 0.45              |
| 57:BY:81:LYS:HD2   | 57:BY:96:ILE:CG2   | 2.46                     | 0.45              |
| 57:BY:7:VAL:HG21   | 57:BY:8:LYS:NZ     | 2.32                     | 0.45              |
| 58:BZ:3:TYR:CD2    | 58:BZ:47:VAL:HG13  | 2.52                     | 0.45              |
| 58:BZ:69:THR:HA    | 58:BZ:89:PHE:O     | 2.16                     | 0.45              |
| 1:CA:1371:G:OP2    | 9:CI:11:LYS:HD2    | 2.17                     | 0.45              |
| 1:CA:256:U:O2'     | 1:CA:257:G:H5'     | 2.17                     | 0.45              |
| 1:CA:32:A:H2'      | 1:CA:33:A:C8       | 2.52                     | 0.45              |
| 2:CB:111:ARG:HG2   | 2:CB:111:ARG:NH1   | 2.32                     | 0.45              |
| 2:CB:55:PHE:HD1    | 2:CB:221:LEU:HG    | 1.82                     | 0.45              |
| 2:CB:52:GLU:O      | 2:CB:56:ARG:HG2    | 2.16                     | 0.45              |
| 3:CC:32:LEU:HD22   | 3:CC:59:ARG:HH12   | 1.82                     | 0.45              |
| 4:CD:101:LEU:HD23  | 4:CD:121:VAL:CG1   | 2.47                     | 0.45              |
| 7:CG:22:LEU:HD23   | 7:CG:22:LEU:O      | 2.15                     | 0.45              |
| 12:CL:17:LYS:HD3   | 12:CL:18:VAL:H     | 1.81                     | 0.45              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 12:CL:38:THR:HG23  | 12:CL:57:LYS:HB3  | 1.99                     | 0.45              |
| 15:CO:3:ILE:HG13   | 15:CO:3:ILE:O     | 2.16                     | 0.45              |
| 17:CQ:52:LYS:HD3   | 17:CQ:55:ASP:OD2  | 2.16                     | 0.45              |
| 19:CS:10:PHE:CE2   | 19:CS:37:ARG:O    | 2.69                     | 0.45              |
| 22:CW:37:U:H2'     | 22:CW:38:A:H8     | 1.81                     | 0.45              |
| 22:CW:52:C:H2'     | 22:CW:53:G:C5'    | 2.46                     | 0.45              |
| 24:CY:164:MET:SD   | 24:CY:216:LEU:CD1 | 3.05                     | 0.45              |
| 24:CY:424:LEU:HD12 | 24:CY:427:ALA:CB  | 2.46                     | 0.45              |
| 24:CY:498:ILE:HG22 | 24:CY:507:TYR:CE2 | 2.52                     | 0.45              |
| 24:CY:530:VAL:HG22 | 24:CY:531:GLY:N   | 2.24                     | 0.45              |
| 26:D1:62:VAL:HG22  | 26:D1:63:ALA:N    | 2.32                     | 0.45              |
| 32:D7:35:ARG:O     | 32:D7:38:GLY:N    | 2.48                     | 0.45              |
| 35:DA:222:A:H5''   | 35:DA:421:U:OP1   | 2.17                     | 0.45              |
| 35:DA:2419:U:O2'   | 35:DA:2420:C:H5'  | 2.16                     | 0.45              |
| 35:DA:2441:C:O2'   | 35:DA:2442:C:H5'  | 2.17                     | 0.45              |
| 35:DA:2604:U:H2'   | 35:DA:2605:U:H6   | 1.81                     | 0.45              |
| 35:DA:26:G:H1'     | 35:DA:515:A:N6    | 2.32                     | 0.45              |
| 35:DA:271(H):G:H1  | 35:DA:271(P):C:N4 | 2.15                     | 0.45              |
| 35:DA:2754:U:C2'   | 35:DA:2755:C:H5'  | 2.47                     | 0.45              |
| 35:DA:2762:G:C8    | 35:DA:2762:G:C5'  | 3.00                     | 0.45              |
| 35:DA:2845:G:H8    | 35:DA:2845:G:O5'  | 2.00                     | 0.45              |
| 35:DA:2836:U:C4    | 35:DA:2883:A:N6   | 2.85                     | 0.45              |
| 35:DA:560:C:H2'    | 35:DA:561:G:O4'   | 2.17                     | 0.45              |
| 35:DA:568:U:H2'    | 35:DA:570:G:OP2   | 2.16                     | 0.45              |
| 35:DA:677:A:H4'    | 35:DA:2070:G:O2'  | 2.16                     | 0.45              |
| 35:DA:686:G:N2     | 35:DA:788:A:H61   | 2.15                     | 0.45              |
| 35:DA:950:G:H2'    | 35:DA:951:C:C6    | 2.52                     | 0.45              |
| 35:DA:963:U:H2'    | 35:DA:964:C:C6    | 2.52                     | 0.45              |
| 36:DB:82:G:C2      | 36:DB:83:G:C8     | 3.05                     | 0.45              |
| 38:DD:34:VAL:CG2   | 38:DD:35:LYS:N    | 2.70                     | 0.45              |
| 40:DF:127:GLU:O    | 40:DF:127:GLU:OE2 | 2.35                     | 0.45              |
| 35:DA:440:G:N2     | 40:DF:46:ARG:NH2  | 2.65                     | 0.45              |
| 29:D4:26:SER:HB3   | 41:DG:105:LYS:NZ  | 2.32                     | 0.45              |
| 43:DJ:94:UNK:O     | 43:DJ:95:UNK:C    | 2.64                     | 0.45              |
| 44:DK:8:VAL:HG12   | 44:DK:10:LEU:HG   | 1.98                     | 0.45              |
| 46:DN:125:GLY:CA   | 46:DN:126:PRO:O   | 2.64                     | 0.45              |
| 49:DQ:59:ARG:O     | 49:DQ:60:ARG:HB2  | 2.17                     | 0.45              |
| 50:DR:18:LEU:HD21  | 50:DR:22:ARG:CZ   | 2.46                     | 0.45              |
| 50:DR:3:HIS:O      | 50:DR:4:LEU:HB3   | 2.16                     | 0.45              |
| 52:DT:29:ARG:HG3   | 52:DT:30:VAL:HG13 | 1.99                     | 0.45              |
| 52:DT:55:ASN:ND2   | 52:DT:55:ASN:O    | 2.49                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 52:DT:45:PHE:HE2   | 52:DT:74:ARG:HB2  | 1.79                     | 0.45              |
| 54:DV:35:LEU:HB3   | 54:DV:37:VAL:CG2  | 2.46                     | 0.45              |
| 35:DA:1341:U:H4'   | 56:DX:57:LEU:HB3  | 1.99                     | 0.45              |
| 57:DY:95:LYS:CE    | 57:DY:101:LYS:H   | 2.30                     | 0.45              |
| 58:DZ:14:LYS:O     | 58:DZ:18:LEU:HD13 | 2.16                     | 0.45              |
| 58:DZ:25:PRO:HA    | 58:DZ:38:TYR:HB2  | 1.98                     | 0.45              |
| 36:DB:76:G:H21     | 58:DZ:75:ASN:ND2  | 2.14                     | 0.45              |
| 58:DZ:82:ARG:O     | 58:DZ:83:PRO:C    | 2.54                     | 0.45              |
| 1:AA:10:A:H2'      | 1:AA:11:G:C8      | 2.52                     | 0.45              |
| 1:AA:322:C:H41     | 1:AA:328:C:H6     | 1.64                     | 0.45              |
| 1:AA:335:C:O2      | 1:AA:1433:A:H2    | 2.00                     | 0.45              |
| 1:AA:96:U:O2'      | 1:AA:97:G:H8      | 2.00                     | 0.45              |
| 1:AA:973:G:O4'     | 10:AJ:55:LYS:CG   | 2.57                     | 0.45              |
| 2:AB:142:LEU:HD23  | 2:AB:142:LEU:O    | 2.17                     | 0.45              |
| 2:AB:208:ILE:O     | 2:AB:212:GLN:HB2  | 2.16                     | 0.45              |
| 2:AB:238:LEU:O     | 2:AB:240:GLN:N    | 2.49                     | 0.45              |
| 3:AC:165:THR:O     | 3:AC:165:THR:HG23 | 2.16                     | 0.45              |
| 14:AN:29:ARG:CG    | 14:AN:29:ARG:HH11 | 2.30                     | 0.45              |
| 18:AR:30:ASP:C     | 18:AR:32:ARG:H    | 2.19                     | 0.45              |
| 22:AV:7:G:H3'      | 22:AV:8:U:H5'     | 1.97                     | 0.45              |
| 22:AW:17:C:O2      | 22:AW:17:C:O4'    | 2.33                     | 0.45              |
| 22:AW:77:A:H61     | 35:BA:2422:A:C5'  | 2.30                     | 0.45              |
| 24:AY:100:VAL:HG22 | 24:AY:101:LEU:N   | 2.32                     | 0.45              |
| 24:AY:191:ASP:N    | 24:AY:191:ASP:OD1 | 2.50                     | 0.45              |
| 24:AY:510:VAL:HA   | 24:AY:570:GLY:HA3 | 1.98                     | 0.45              |
| 24:AY:491:VAL:CG1  | 24:AY:596:LYS:HD3 | 2.44                     | 0.45              |
| 26:B1:64:ALA:C     | 26:B1:66:HIS:N    | 2.70                     | 0.45              |
| 26:B1:82:LEU:C     | 26:B1:83:GLU:HG3  | 2.37                     | 0.45              |
| 27:B2:48:HIS:O     | 27:B2:50:ILE:N    | 2.49                     | 0.45              |
| 27:B2:32:LEU:HD11  | 27:B2:54:LYS:HG2  | 1.98                     | 0.45              |
| 28:B3:44:ARG:O     | 28:B3:45:GLY:C    | 2.54                     | 0.45              |
| 33:B8:36:LYS:O     | 33:B8:37:SER:C    | 2.55                     | 0.45              |
| 35:BA:1236:G:HO2'  | 35:BA:1237:A:H8   | 1.63                     | 0.45              |
| 35:BA:1578:U:O2    | 35:BA:1578:U:H2'  | 2.15                     | 0.45              |
| 35:BA:1771:C:H2'   | 35:BA:1772:G:H8   | 1.81                     | 0.45              |
| 35:BA:1840:G:H1    | 35:BA:1902:C:N4   | 2.15                     | 0.45              |
| 35:BA:2086:U:H2'   | 35:BA:2087:G:C8   | 2.52                     | 0.45              |
| 35:BA:2369:A:H2'   | 35:BA:2370:G:H8   | 1.82                     | 0.45              |
| 35:BA:41:C:N4      | 35:BA:437:G:H1    | 2.15                     | 0.45              |
| 35:BA:438:G:H2'    | 35:BA:440:G:C8    | 2.52                     | 0.45              |
| 39:BE:132:HIS:CG   | 39:BE:135:HIS:NE2 | 2.84                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:BE:103:ASP:CG   | 39:BE:201:THR:HA   | 2.38                     | 0.45              |
| 39:BE:93:VAL:O     | 39:BE:95:ILE:N     | 2.50                     | 0.45              |
| 39:BE:9:VAL:HG22   | 39:BE:25:VAL:HB    | 1.99                     | 0.45              |
| 42:BH:61:HIS:O     | 42:BH:62:LYS:C     | 2.55                     | 0.45              |
| 47:BO:61:VAL:N     | 47:BO:87:ILE:HD11  | 2.32                     | 0.45              |
| 49:BQ:108:GLY:C    | 49:BQ:109:VAL:HG23 | 2.37                     | 0.45              |
| 50:BR:41:ALA:O     | 50:BR:43:GLU:N     | 2.50                     | 0.45              |
| 52:BT:108:ARG:CG   | 52:BT:109:GLU:N    | 2.74                     | 0.45              |
| 52:BT:29:ARG:O     | 52:BT:30:VAL:O     | 2.34                     | 0.45              |
| 39:BE:181:LEU:HD11 | 52:BT:7:ILE:HG21   | 1.99                     | 0.45              |
| 52:BT:93:ARG:HD2   | 52:BT:93:ARG:HA    | 1.76                     | 0.45              |
| 53:BU:106:PHE:HA   | 53:BU:109:LEU:HD12 | 1.99                     | 0.45              |
| 55:BW:8:ARG:HA     | 55:BW:102:HIS:HA   | 1.99                     | 0.45              |
| 55:BW:25:ARG:HB2   | 55:BW:25:ARG:NH1   | 2.31                     | 0.45              |
| 55:BW:66:GLU:HG3   | 55:BW:69:LEU:HD12  | 1.97                     | 0.45              |
| 57:BY:77:PRO:HB2   | 57:BY:99:CYS:SG    | 2.57                     | 0.45              |
| 1:CA:1095:U:OP1    | 1:CA:1108:G:N2     | 2.49                     | 0.45              |
| 1:CA:1225:A:H5'    | 1:CA:1226:C:OP2    | 2.17                     | 0.45              |
| 1:CA:155:C:H2'     | 1:CA:156:G:C8      | 2.52                     | 0.45              |
| 1:CA:545:C:O2'     | 1:CA:546:G:H5'     | 2.17                     | 0.45              |
| 1:CA:693:G:C5      | 23:CX:13:A:H1'     | 2.52                     | 0.45              |
| 2:CB:24:TRP:HA     | 2:CB:190:THR:O     | 2.17                     | 0.45              |
| 2:CB:88:ALA:HB2    | 2:CB:219:VAL:CG1   | 2.45                     | 0.45              |
| 3:CC:84:ILE:O      | 3:CC:84:ILE:HG12   | 2.16                     | 0.45              |
| 4:CD:110:PHE:CD1   | 4:CD:110:PHE:N     | 2.84                     | 0.45              |
| 4:CD:168:ARG:N     | 4:CD:168:ARG:HD2   | 2.32                     | 0.45              |
| 7:CG:102:ARG:HG2   | 7:CG:106:GLN:HE21  | 1.78                     | 0.45              |
| 7:CG:80:VAL:CG2    | 7:CG:81:GLY:H      | 2.27                     | 0.45              |
| 8:CH:34:GLU:O      | 8:CH:35:ILE:C      | 2.54                     | 0.45              |
| 11:CK:33:THR:HB    | 11:CK:38:ASN:C     | 2.37                     | 0.45              |
| 6:CF:100:ASN:O     | 18:CR:28:GLU:HG2   | 2.16                     | 0.45              |
| 19:CS:58:VAL:O     | 19:CS:60:VAL:N     | 2.50                     | 0.45              |
| 24:CY:145:ASP:OD2  | 24:CY:148:LEU:HB2  | 2.17                     | 0.45              |
| 24:CY:206:LEU:HD12 | 24:CY:210:ARG:HH12 | 1.82                     | 0.45              |
| 24:CY:358:MET:SD   | 24:CY:363:ARG:HG2  | 2.56                     | 0.45              |
| 24:CY:428:LEU:HD13 | 24:CY:440:VAL:HG21 | 1.99                     | 0.45              |
| 24:CY:453:GLY:HA2  | 24:CY:458:HIS:CD2  | 2.52                     | 0.45              |
| 24:CY:517:LEU:HD11 | 24:CY:564:LYS:CB   | 2.43                     | 0.45              |
| 25:D0:20:ARG:CG    | 25:D0:20:ARG:HH11  | 2.30                     | 0.45              |
| 27:D2:37:PHE:O     | 27:D2:41:ILE:HG23  | 2.17                     | 0.45              |
| 28:D3:46:ASN:O     | 28:D3:47:VAL:C     | 2.54                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:1045:A:O2'   | 35:DA:1047:G:C5    | 2.66                     | 0.45              |
| 35:DA:1052:C:C6    | 35:DA:1052:C:H3'   | 2.52                     | 0.45              |
| 35:DA:1052:C:P     | 35:DA:1052:C:O4'   | 2.74                     | 0.45              |
| 35:DA:1328:G:H2'   | 35:DA:1330:C:C4    | 2.51                     | 0.45              |
| 35:DA:1331:A:C2'   | 35:DA:1332:G:H5''  | 2.46                     | 0.45              |
| 35:DA:1487:G:H2'   | 35:DA:1487:G:N3    | 2.32                     | 0.45              |
| 35:DA:1464:C:O2'   | 35:DA:1528:A:C8    | 2.66                     | 0.45              |
| 35:DA:1578:U:O2    | 35:DA:1578:U:H2'   | 2.17                     | 0.45              |
| 35:DA:1609:A:H1'   | 35:DA:1616:A:H1'   | 1.98                     | 0.45              |
| 35:DA:1682:G:O2'   | 35:DA:1683:C:H5'   | 2.17                     | 0.45              |
| 35:DA:1813:G:H1'   | 38:DD:50:THR:OG1   | 2.17                     | 0.45              |
| 35:DA:1825:A:OP1   | 38:DD:249:PRO:HD3  | 2.17                     | 0.45              |
| 35:DA:1917:U:H2'   | 35:DA:1918:A:H5'   | 1.97                     | 0.45              |
| 35:DA:1943:U:C2'   | 35:DA:1943:U:O2    | 2.64                     | 0.45              |
| 35:DA:1935:G:H1'   | 35:DA:1964:G:N2    | 2.31                     | 0.45              |
| 35:DA:214:G:H2'    | 35:DA:215:G:O4'    | 2.17                     | 0.45              |
| 35:DA:2163:C:C2'   | 35:DA:2164:C:H5'   | 2.47                     | 0.45              |
| 22:CW:77:A:O2'     | 35:DA:2394:C:N3    | 2.40                     | 0.45              |
| 35:DA:2552:U:O5'   | 35:DA:2552:U:H6    | 1.99                     | 0.45              |
| 35:DA:2712:U:H2'   | 35:DA:2713:A:H5'   | 1.98                     | 0.45              |
| 35:DA:2809:A:C2    | 35:DA:2892:A:N3    | 2.84                     | 0.45              |
| 35:DA:2881:C:C2    | 35:DA:2882:A:C8    | 3.05                     | 0.45              |
| 35:DA:626:U:H3     | 48:DP:105:LEU:HG   | 1.82                     | 0.45              |
| 35:DA:654(P):C:O2' | 35:DA:654(Q):C:H5' | 2.17                     | 0.45              |
| 35:DA:654(R):C:O2' | 35:DA:654(S):G:H8  | 1.98                     | 0.45              |
| 35:DA:74:A:H5''    | 35:DA:75:G:O4'     | 2.16                     | 0.45              |
| 35:DA:864:G:H21    | 35:DA:866:A:H61    | 1.65                     | 0.45              |
| 36:DB:106:G:O2'    | 36:DB:107:G:H5'    | 2.16                     | 0.45              |
| 36:DB:64:C:O2'     | 36:DB:65:C:H5'     | 2.17                     | 0.45              |
| 35:DA:2787:C:H1'   | 39:DE:61:ARG:HD3   | 1.99                     | 0.45              |
| 40:DF:201:VAL:HA   | 40:DF:204:ASN:HD22 | 1.82                     | 0.45              |
| 40:DF:31:HIS:O     | 40:DF:34:TRP:HB3   | 2.17                     | 0.45              |
| 40:DF:83:PHE:O     | 40:DF:84:VAL:C     | 2.53                     | 0.45              |
| 42:DH:94:TYR:CD2   | 42:DH:107:VAL:HG12 | 2.52                     | 0.45              |
| 44:DK:62:ASP:O     | 44:DK:63:ARG:HB2   | 2.16                     | 0.45              |
| 48:DP:122:PRO:O    | 48:DP:123:LEU:HD23 | 2.16                     | 0.45              |
| 50:DR:59:ASP:O     | 50:DR:60:LEU:C     | 2.56                     | 0.45              |
| 51:DS:77:ALA:HB1   | 51:DS:82:ILE:HB    | 1.99                     | 0.45              |
| 53:DU:96:ALA:C     | 53:DU:98:LEU:H     | 2.20                     | 0.45              |
| 54:DV:64:HIS:ND1   | 54:DV:92:THR:CG2   | 2.80                     | 0.45              |
| 58:DZ:102:LEU:HG   | 58:DZ:122:ARG:O    | 2.16                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:1195:C:H2'    | 1:AA:1197:G:O4'   | 2.17                     | 0.45              |
| 1:AA:1237:C:H3'    | 1:AA:1336:C:H41   | 1.82                     | 0.45              |
| 1:AA:1499:A:O2'    | 1:AA:1500:A:H5'   | 2.17                     | 0.45              |
| 1:AA:1505:G:C8     | 1:AA:1505:G:H5''  | 2.51                     | 0.45              |
| 1:AA:356:A:H1'     | 1:AA:368:U:O2'    | 2.16                     | 0.45              |
| 1:AA:811:C:H4'     | 1:AA:900:A:N6     | 2.32                     | 0.45              |
| 1:AA:923:A:H2'     | 1:AA:924:C:C6     | 2.51                     | 0.45              |
| 2:AB:97:TRP:CZ3    | 2:AB:173:ALA:HA   | 2.52                     | 0.45              |
| 2:AB:48:MET:HA     | 2:AB:51:LEU:HD12  | 1.99                     | 0.45              |
| 3:AC:83:ARG:C      | 3:AC:85:ARG:N     | 2.68                     | 0.45              |
| 4:AD:168:ARG:HA    | 4:AD:168:ARG:HH11 | 1.81                     | 0.45              |
| 5:AE:8:GLU:HA      | 5:AE:34:VAL:HA    | 1.98                     | 0.45              |
| 12:AL:41:ARG:NH1   | 12:AL:41:ARG:CB   | 2.78                     | 0.45              |
| 19:AS:15:LEU:O     | 19:AS:19:VAL:N    | 2.50                     | 0.45              |
| 19:AS:50:ALA:O     | 19:AS:51:VAL:C    | 2.56                     | 0.45              |
| 24:AY:124:GLN:C    | 24:AY:127:LYS:HB3 | 2.37                     | 0.45              |
| 24:AY:465:ARG:O    | 24:AY:470:PHE:HD2 | 1.99                     | 0.45              |
| 24:AY:497:PHE:O    | 24:AY:498:ILE:O   | 2.35                     | 0.45              |
| 27:B2:13:ALA:C     | 27:B2:15:LYS:N    | 2.69                     | 0.45              |
| 27:B2:55:ARG:HH21  | 27:B2:55:ARG:HG3  | 1.82                     | 0.45              |
| 33:B8:53:PRO:HG2   | 33:B8:54:GLU:N    | 2.31                     | 0.45              |
| 34:B9:2:LYS:HE3    | 34:B9:2:LYS:HB3   | 1.87                     | 0.45              |
| 35:BA:1452:A:C3'   | 35:BA:1453:U:C5'  | 2.72                     | 0.45              |
| 35:BA:1495:A:N3    | 35:BA:1496:A:C2   | 2.85                     | 0.45              |
| 35:BA:1499:C:C2'   | 35:BA:1500:G:H5'  | 2.46                     | 0.45              |
| 35:BA:2337:G:H2'   | 35:BA:2338:G:C8   | 2.52                     | 0.45              |
| 35:BA:2473:U:C3'   | 35:BA:2474:C:H5'' | 2.16                     | 0.45              |
| 30:B5:3:LYS:CE     | 35:BA:2613:U:H2'  | 2.47                     | 0.45              |
| 35:BA:271(C):C:H2' | 35:BA:271(D):G:H8 | 1.81                     | 0.45              |
| 35:BA:2762:G:H8    | 35:BA:2762:G:C5'  | 2.28                     | 0.45              |
| 35:BA:2887:U:H2'   | 35:BA:2888:C:C6   | 2.52                     | 0.45              |
| 35:BA:288:C:O2'    | 35:BA:289:A:H5'   | 2.17                     | 0.45              |
| 35:BA:299:A:H1'    | 35:BA:322:A:N6    | 2.32                     | 0.45              |
| 35:BA:338:G:O2'    | 35:BA:339:U:H5'   | 2.16                     | 0.45              |
| 35:BA:389:G:O4'    | 35:BA:2413:G:C4'  | 2.65                     | 0.45              |
| 35:BA:492:A:H2'    | 35:BA:493:G:C5'   | 2.46                     | 0.45              |
| 35:BA:657:U:C2     | 35:BA:658:C:C5    | 3.05                     | 0.45              |
| 35:BA:686:G:N2     | 35:BA:788:A:H61   | 2.15                     | 0.45              |
| 35:BA:74:A:H5''    | 35:BA:75:G:O4'    | 2.17                     | 0.45              |
| 37:BC:173:HIS:O    | 37:BC:174:ALA:HB2 | 2.16                     | 0.45              |
| 35:BA:782:A:C2     | 38:BD:226:MET:HG2 | 2.51                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:BD:31:LYS:HZ2   | 38:BD:33:LEU:HB2   | 1.81                     | 0.45              |
| 38:BD:43:ARG:NH1   | 38:BD:49:ILE:HG22  | 2.31                     | 0.45              |
| 40:BF:126:VAL:HG23 | 40:BF:127:GLU:N    | 2.32                     | 0.45              |
| 40:BF:157:VAL:HG23 | 40:BF:157:VAL:O    | 2.16                     | 0.45              |
| 40:BF:160:ASN:ND2  | 40:BF:162:LEU:HB2  | 2.28                     | 0.45              |
| 41:BG:16:ARG:HH11  | 41:BG:16:ARG:HG3   | 1.82                     | 0.45              |
| 41:BG:67:LYS:CD    | 41:BG:68:PRO:O     | 2.65                     | 0.45              |
| 43:BJ:67:UNK:C     | 43:BJ:69:UNK:N     | 2.80                     | 0.45              |
| 46:BN:104:LYS:HB2  | 46:BN:117:PHE:CE1  | 2.52                     | 0.45              |
| 46:BN:55:VAL:HG22  | 46:BN:56:ASN:N     | 2.32                     | 0.45              |
| 47:BO:91:LEU:N     | 47:BO:91:LEU:CD2   | 2.79                     | 0.45              |
| 48:BP:133:SER:O    | 48:BP:136:GLU:HG2  | 2.17                     | 0.45              |
| 52:BT:55:ASN:ND2   | 52:BT:58:ASN:HD21  | 2.15                     | 0.45              |
| 53:BU:83:LEU:CD1   | 53:BU:113:ALA:HB2  | 2.47                     | 0.45              |
| 53:BU:83:LEU:HG    | 53:BU:88:ILE:HD11  | 1.98                     | 0.45              |
| 55:BW:66:GLU:HA    | 55:BW:69:LEU:HD12  | 1.97                     | 0.45              |
| 56:BX:71:GLY:C     | 56:BX:72:LYS:HG3   | 2.37                     | 0.45              |
| 57:BY:10:GLY:C     | 57:BY:27:VAL:HG22  | 2.37                     | 0.45              |
| 57:BY:91:GLU:HB2   | 57:BY:92:ASN:H     | 1.57                     | 0.45              |
| 58:BZ:141:VAL:O    | 58:BZ:142:SER:CB   | 2.64                     | 0.45              |
| 1:CA:1225:A:N3     | 1:CA:1225:A:C2'    | 2.77                     | 0.45              |
| 1:CA:1314:C:N4     | 19:CS:4:SER:N      | 2.65                     | 0.45              |
| 1:CA:238:G:O2'     | 1:CA:239:U:H5'     | 2.17                     | 0.45              |
| 1:CA:883:C:O2'     | 1:CA:884:U:H5'     | 2.17                     | 0.45              |
| 2:CB:189:ASP:OD2   | 2:CB:205:ASP:OD1   | 2.35                     | 0.45              |
| 3:CC:112:SER:OG    | 3:CC:114:PRO:HD2   | 2.17                     | 0.45              |
| 3:CC:155:GLY:O     | 3:CC:156:ARG:HB2   | 2.17                     | 0.45              |
| 4:CD:163:GLU:HA    | 4:CD:163:GLU:OE2   | 2.15                     | 0.45              |
| 8:CH:32:LYS:O      | 8:CH:34:GLU:N      | 2.50                     | 0.45              |
| 11:CK:24:SER:O     | 11:CK:88:GLY:HA2   | 2.17                     | 0.45              |
| 12:CL:30:ALA:CB    | 12:CL:33:ARG:HH21  | 2.30                     | 0.45              |
| 18:CR:44:LEU:O     | 18:CR:45:SER:O     | 2.34                     | 0.45              |
| 19:CS:15:LEU:O     | 19:CS:19:VAL:N     | 2.50                     | 0.45              |
| 20:CT:16:HIS:O     | 20:CT:17:ARG:C     | 2.55                     | 0.45              |
| 24:CY:182:ARG:C    | 24:CY:184:LYS:H    | 2.21                     | 0.45              |
| 24:CY:293:THR:C    | 24:CY:295:GLU:N    | 2.67                     | 0.45              |
| 24:CY:613:PRO:CG   | 24:CY:666:ARG:HH21 | 2.30                     | 0.45              |
| 26:D1:82:LEU:HD23  | 26:D1:90:ILE:HD12  | 1.98                     | 0.45              |
| 28:D3:19:GLN:O     | 28:D3:22:ALA:HB3   | 2.16                     | 0.45              |
| 29:D4:21:VAL:HG12  | 29:D4:21:VAL:O     | 2.16                     | 0.45              |
| 29:D4:39:CYS:SG    | 29:D4:42:PHE:HE2   | 2.40                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:D4:43:TYR:CD2  | 29:D4:44:THR:HG23  | 2.52                     | 0.45              |
| 30:D5:59:GLU:HB3  | 30:D5:60:VAL:H     | 1.68                     | 0.45              |
| 33:D8:29:LYS:HD2  | 33:D8:44:LYS:HG2   | 1.99                     | 0.45              |
| 35:DA:1009:A:H1'  | 53:DU:59:ARG:NH1   | 2.32                     | 0.45              |
| 35:DA:1472:A:H2'  | 35:DA:1473:G:C8    | 2.52                     | 0.45              |
| 35:DA:1478:G:HO2' | 35:DA:1558:A:H2    | 1.64                     | 0.45              |
| 35:DA:15:G:H2'    | 35:DA:16:G:H8      | 1.81                     | 0.45              |
| 35:DA:17:G:H2'    | 35:DA:18:C:C6      | 2.52                     | 0.45              |
| 26:D1:45:ASN:ND2  | 35:DA:2090:G:H21   | 2.07                     | 0.45              |
| 35:DA:2126:A:H1'  | 35:DA:2127:G:O4'   | 2.17                     | 0.45              |
| 35:DA:2555:U:C2'  | 35:DA:2556:C:H5'   | 2.47                     | 0.45              |
| 35:DA:42:G:N3     | 35:DA:42:G:H2'     | 2.32                     | 0.45              |
| 35:DA:496:G:C6    | 35:DA:497:A:C4     | 3.05                     | 0.45              |
| 35:DA:949:C:H2'   | 35:DA:950:G:H8     | 1.81                     | 0.45              |
| 35:DA:960:A:C8    | 35:DA:962:G:C8     | 3.04                     | 0.45              |
| 36:DB:89:G:C6     | 36:DB:90:A:N1      | 2.85                     | 0.45              |
| 38:DD:48:ARG:HG3  | 38:DD:48:ARG:HH11  | 1.81                     | 0.45              |
| 40:DF:107:LYS:HD2 | 40:DF:205:ARG:O    | 2.16                     | 0.45              |
| 41:DG:57:ALA:HA   | 41:DG:90:LEU:HD22  | 1.99                     | 0.45              |
| 44:DK:103:GLN:HA  | 44:DK:106:GLU:OE2  | 2.17                     | 0.45              |
| 46:DN:57:ALA:O    | 46:DN:58:ASP:C     | 2.53                     | 0.45              |
| 48:DP:122:PRO:HA  | 48:DP:141:ALA:O    | 2.17                     | 0.45              |
| 50:DR:11:ASN:O    | 50:DR:12:ARG:CB    | 2.64                     | 0.45              |
| 51:DS:87:PHE:HB2  | 51:DS:106:ARG:HH21 | 1.82                     | 0.45              |
| 52:DT:113:LYS:O   | 52:DT:114:LEU:HD23 | 2.17                     | 0.45              |
| 53:DU:115:ALA:C   | 53:DU:117:GLN:N    | 2.70                     | 0.45              |
| 53:DU:21:ALA:HA   | 53:DU:24:TYR:CD1   | 2.52                     | 0.45              |
| 53:DU:50:ARG:C    | 53:DU:52:ARG:N     | 2.69                     | 0.45              |
| 54:DV:47:VAL:O    | 54:DV:47:VAL:HG23  | 2.16                     | 0.45              |
| 57:DY:39:VAL:O    | 57:DY:40:GLU:CD    | 2.55                     | 0.45              |
| 58:DZ:153:SER:O   | 58:DZ:155:LEU:HD23 | 2.16                     | 0.45              |
| 1:AA:115:G:H1'    | 1:AA:116:A:N7      | 2.32                     | 0.44              |
| 1:AA:1225:A:N3    | 1:AA:1225:A:C2'    | 2.77                     | 0.44              |
| 1:AA:1300:G:O2'   | 1:AA:1301:U:OP2    | 2.35                     | 0.44              |
| 1:AA:1347:G:H2'   | 1:AA:1373:G:C6     | 2.52                     | 0.44              |
| 1:AA:315:A:O2'    | 1:AA:316:G:P       | 2.75                     | 0.44              |
| 1:AA:979:C:C3'    | 1:AA:980:C:C5'     | 2.76                     | 0.44              |
| 3:AC:32:LEU:O     | 3:AC:35:GLU:HB3    | 2.17                     | 0.44              |
| 3:AC:35:GLU:OE1   | 3:AC:97:LYS:HE3    | 2.17                     | 0.44              |
| 4:AD:199:ASN:OD1  | 4:AD:201:GLN:HB2   | 2.17                     | 0.44              |
| 5:AE:129:ILE:O    | 5:AE:132:ALA:HB3   | 2.17                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 5:AE:8:GLU:CA      | 5:AE:34:VAL:HG23  | 2.46                     | 0.44              |
| 5:AE:9:LYS:NZ      | 5:AE:111:GLU:OE1  | 2.50                     | 0.44              |
| 6:AF:62:TRP:CE2    | 18:AR:35:ARG:NH2  | 2.85                     | 0.44              |
| 1:AA:778:G:H1'     | 11:AK:119:CYS:HB3 | 1.98                     | 0.44              |
| 12:AL:39:VAL:HG21  | 12:AL:57:LYS:HD2  | 1.99                     | 0.44              |
| 13:AM:37:THR:HG21  | 13:AM:56:LEU:HA   | 1.97                     | 0.44              |
| 13:AM:79:LYS:HA    | 13:AM:82:MET:CG   | 2.47                     | 0.44              |
| 15:AO:50:HIS:O     | 15:AO:53:HIS:HB3  | 2.16                     | 0.44              |
| 6:AF:60:PHE:CE2    | 18:AR:78:LEU:HD21 | 2.52                     | 0.44              |
| 1:AA:1221:G:P      | 19:AS:36:ARG:HD3  | 2.56                     | 0.44              |
| 22:AW:37:U:N3      | 23:AX:13:A:N6     | 2.65                     | 0.44              |
| 24:AY:302:HIS:HA   | 24:AY:303:PRO:HD2 | 1.74                     | 0.44              |
| 24:AY:14:ASN:ND2   | 24:AY:80:ASN:HD22 | 2.14                     | 0.44              |
| 26:B1:53:VAL:O     | 26:B1:54:ALA:C    | 2.54                     | 0.44              |
| 27:B2:13:ALA:O     | 27:B2:15:LYS:N    | 2.50                     | 0.44              |
| 35:BA:1331:A:O2'   | 35:BA:1332:G:H8   | 2.00                     | 0.44              |
| 35:BA:1381:G:N2    | 35:BA:1382:G:H1'  | 2.32                     | 0.44              |
| 35:BA:1416:G:H1'   | 35:BA:1417:C:C5   | 2.52                     | 0.44              |
| 35:BA:1826:G:H2'   | 35:BA:1827:C:H6   | 1.82                     | 0.44              |
| 35:BA:1856:G:H1    | 35:BA:1886:C:H42  | 1.64                     | 0.44              |
| 35:BA:2650:U:O2'   | 35:BA:2651:C:H5'  | 2.17                     | 0.44              |
| 35:BA:333:G:N3     | 35:BA:333:G:H2'   | 2.32                     | 0.44              |
| 35:BA:526:A:N6     | 35:BA:2626:C:H4'  | 2.32                     | 0.44              |
| 35:BA:625:G:H5'    | 35:BA:657:U:OP1   | 2.17                     | 0.44              |
| 35:BA:703:U:O2'    | 35:BA:704:G:H5'   | 2.17                     | 0.44              |
| 36:BB:14:U:H5'     | 36:BB:71:C:O4'    | 2.16                     | 0.44              |
| 36:BB:86:G:H2'     | 36:BB:87:G:H8     | 1.77                     | 0.44              |
| 40:BF:165:ARG:HH11 | 40:BF:165:ARG:HB3 | 1.82                     | 0.44              |
| 41:BG:8:LYS:O      | 41:BG:12:TYR:HD1  | 2.00                     | 0.44              |
| 41:BG:67:LYS:HD3   | 41:BG:68:PRO:O    | 2.16                     | 0.44              |
| 44:BK:21:PRO:HA    | 44:BK:23:VAL:H    | 1.82                     | 0.44              |
| 46:BN:133:GLN:CG   | 46:BN:134:ARG:H   | 2.30                     | 0.44              |
| 47:BO:24:VAL:HG23  | 47:BO:24:VAL:O    | 2.16                     | 0.44              |
| 50:BR:106:GLY:O    | 50:BR:107:ASP:HB3 | 2.16                     | 0.44              |
| 50:BR:94:TYR:CD1   | 50:BR:94:TYR:N    | 2.85                     | 0.44              |
| 51:BS:12:PHE:HD1   | 51:BS:12:PHE:C    | 2.20                     | 0.44              |
| 51:BS:65:VAL:C     | 51:BS:67:ARG:H    | 2.20                     | 0.44              |
| 53:BU:33:ARG:C     | 53:BU:35:ALA:H    | 2.20                     | 0.44              |
| 1:CA:197:A:H4'     | 1:CA:198:G:H5'    | 1.98                     | 0.44              |
| 1:CA:605:U:O2'     | 1:CA:606:G:H5'    | 2.17                     | 0.44              |
| 1:CA:781:A:C2'     | 1:CA:782:A:H5'    | 2.47                     | 0.44              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:826:C:H2'     | 1:CA:827:U:H6      | 1.81                     | 0.44              |
| 3:CC:182:ILE:HG12  | 3:CC:203:PHE:HD1   | 1.81                     | 0.44              |
| 3:CC:25:GLY:C      | 3:CC:27:LYS:N      | 2.70                     | 0.44              |
| 3:CC:83:ARG:C      | 3:CC:85:ARG:H      | 2.21                     | 0.44              |
| 6:CF:62:TRP:CD1    | 18:CR:35:ARG:NH1   | 2.85                     | 0.44              |
| 10:CJ:4:ILE:CB     | 10:CJ:74:ILE:HD11  | 2.48                     | 0.44              |
| 11:CK:33:THR:HG22  | 11:CK:39:PRO:CA    | 2.40                     | 0.44              |
| 12:CL:28:LYS:HB2   | 12:CL:33:ARG:HH22  | 1.82                     | 0.44              |
| 13:CM:3:ARG:HH21   | 13:CM:7:VAL:HG13   | 1.82                     | 0.44              |
| 20:CT:30:LYS:HZ2   | 20:CT:34:LYS:HE3   | 1.81                     | 0.44              |
| 24:CY:122:TRP:C    | 24:CY:124:GLN:N    | 2.69                     | 0.44              |
| 24:CY:162:VAL:CG1  | 24:CY:216:LEU:HD12 | 2.47                     | 0.44              |
| 24:CY:457:LEU:O    | 24:CY:458:HIS:C    | 2.55                     | 0.44              |
| 24:CY:414:GLU:O    | 24:CY:474:ALA:HB1  | 2.17                     | 0.44              |
| 29:D4:51:ASP:OD2   | 29:D4:52:THR:HG23  | 2.17                     | 0.44              |
| 35:DA:1114:G:H2'   | 35:DA:1115:G:C5'   | 2.47                     | 0.44              |
| 35:DA:1411:C:N4    | 35:DA:1412:A:N6    | 2.66                     | 0.44              |
| 35:DA:1491:G:H2'   | 35:DA:1491:G:N3    | 2.33                     | 0.44              |
| 35:DA:1555:G:N3    | 35:DA:1555:G:H2'   | 2.32                     | 0.44              |
| 35:DA:1799:G:N2    | 35:DA:1818:U:H2'   | 2.32                     | 0.44              |
| 35:DA:1799:G:H5'   | 35:DA:1819:A:H61   | 1.81                     | 0.44              |
| 35:DA:1947:C:H2'   | 35:DA:1948:G:H8    | 1.83                     | 0.44              |
| 35:DA:45:C:OP2     | 35:DA:215:G:H5'    | 2.17                     | 0.44              |
| 35:DA:216:A:H2'    | 35:DA:217:G:H8     | 1.81                     | 0.44              |
| 35:DA:269:U:H2'    | 35:DA:270:A:H8     | 1.81                     | 0.44              |
| 35:DA:331:A:O2'    | 35:DA:332:A:OP1    | 2.26                     | 0.44              |
| 35:DA:558:G:C5'    | 46:DN:112:LEU:HD22 | 2.47                     | 0.44              |
| 35:DA:581:C:C2     | 35:DA:582:G:N7     | 2.85                     | 0.44              |
| 35:DA:958:U:H6     | 35:DA:958:U:H3'    | 1.82                     | 0.44              |
| 27:D2:48:HIS:CE1   | 35:DA:95:G:HO2'    | 2.32                     | 0.44              |
| 38:DD:153:ALA:O    | 38:DD:154:LYS:CG   | 2.65                     | 0.44              |
| 40:DF:10:PRO:HD2   | 40:DF:13:SER:O     | 2.17                     | 0.44              |
| 40:DF:112:MET:HA   | 40:DF:115:ALA:HB3  | 1.99                     | 0.44              |
| 40:DF:192:LEU:C    | 40:DF:192:LEU:CD2  | 2.85                     | 0.44              |
| 42:DH:121:ILE:HD13 | 42:DH:144:VAL:HG21 | 1.99                     | 0.44              |
| 42:DH:54:ARG:HH11  | 42:DH:54:ARG:HG2   | 1.82                     | 0.44              |
| 46:DN:40:PRO:O     | 53:DU:64:ARG:NH2   | 2.49                     | 0.44              |
| 49:DQ:76:LYS:HE2   | 49:DQ:77:LYS:O     | 2.18                     | 0.44              |
| 36:DB:115:G:O4'    | 51:DS:47:THR:HB    | 2.17                     | 0.44              |
| 54:DV:40:LEU:CA    | 54:DV:45:THR:HB    | 2.42                     | 0.44              |
| 57:DY:84:ARG:HG2   | 57:DY:85:VAL:H     | 1.83                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 57:DY:81:LYS:HD2   | 57:DY:96:ILE:CG2  | 2.47                     | 0.44              |
| 1:AA:1004:A:H5'    | 1:AA:1025:U:C4    | 2.52                     | 0.44              |
| 1:AA:1132:C:N4     | 1:AA:1133:G:C6    | 2.85                     | 0.44              |
| 1:AA:1218:C:H2'    | 1:AA:1219:U:C5    | 2.52                     | 0.44              |
| 1:AA:960:U:C6      | 1:AA:1225:A:C8    | 3.05                     | 0.44              |
| 1:AA:1347:G:H2'    | 1:AA:1373:G:O6    | 2.17                     | 0.44              |
| 1:AA:1427:U:H2'    | 1:AA:1428:A:C8    | 2.53                     | 0.44              |
| 1:AA:260:G:O2'     | 1:AA:261:U:H5'    | 2.17                     | 0.44              |
| 1:AA:608:A:C2'     | 1:AA:609:A:H5'    | 2.47                     | 0.44              |
| 1:AA:59:A:H5''     | 1:AA:60:A:H5'     | 1.97                     | 0.44              |
| 1:AA:781:A:C3'     | 1:AA:782:A:H5'    | 2.48                     | 0.44              |
| 1:AA:909:A:H2'     | 1:AA:910:C:O4'    | 2.17                     | 0.44              |
| 2:AB:187:LEU:HD22  | 2:AB:201:ILE:O    | 2.17                     | 0.44              |
| 3:AC:70:VAL:CG1    | 3:AC:71:ALA:N     | 2.62                     | 0.44              |
| 4:AD:163:GLU:C     | 4:AD:165:MET:H    | 2.21                     | 0.44              |
| 5:AE:150:ARG:HB2   | 5:AE:150:ARG:NH1  | 2.32                     | 0.44              |
| 5:AE:29:GLY:HA2    | 5:AE:46:GLY:O     | 2.17                     | 0.44              |
| 5:AE:82:VAL:HG21   | 5:AE:138:ALA:CA   | 2.43                     | 0.44              |
| 7:AG:113:GLU:CG    | 7:AG:119:ARG:HG2  | 2.47                     | 0.44              |
| 9:AI:104:ARG:O     | 9:AI:105:ASP:N    | 2.50                     | 0.44              |
| 9:AI:70:LYS:O      | 9:AI:74:ILE:HG13  | 2.16                     | 0.44              |
| 9:AI:73:GLN:O      | 9:AI:75:ASP:N     | 2.50                     | 0.44              |
| 12:AL:17:LYS:HD3   | 12:AL:18:VAL:H    | 1.82                     | 0.44              |
| 12:AL:18:VAL:O     | 12:AL:19:ARG:CB   | 2.65                     | 0.44              |
| 16:AP:20:VAL:HG22  | 16:AP:21:VAL:N    | 2.32                     | 0.44              |
| 17:AQ:9:VAL:CG1    | 17:AQ:56:VAL:HG22 | 2.47                     | 0.44              |
| 19:AS:35:SER:C     | 19:AS:37:ARG:H    | 2.19                     | 0.44              |
| 19:AS:5:LEU:HD12   | 19:AS:8:GLY:C     | 2.36                     | 0.44              |
| 21:AU:2:GLY:C      | 21:AU:4:GLY:N     | 2.70                     | 0.44              |
| 22:AV:32:C:C4      | 22:AV:33:U:C5     | 3.05                     | 0.44              |
| 24:AY:181:LEU:HD23 | 24:AY:182:ARG:NH1 | 2.33                     | 0.44              |
| 24:AY:262:SER:OG   | 24:AY:265:LYS:HG3 | 2.17                     | 0.44              |
| 24:AY:435:ASP:OD2  | 24:AY:435:ASP:C   | 2.55                     | 0.44              |
| 28:B3:8:LEU:O      | 28:B3:31:LEU:HD22 | 2.17                     | 0.44              |
| 31:B6:15:GLU:OE1   | 31:B6:41:PRO:HG3  | 2.18                     | 0.44              |
| 35:BA:55:G:H1      | 35:BA:115:C:H42   | 1.65                     | 0.44              |
| 35:BA:1511:C:H2'   | 35:BA:1512:U:O4'  | 2.16                     | 0.44              |
| 35:BA:1530:C:H2'   | 35:BA:1531:C:H6   | 1.83                     | 0.44              |
| 35:BA:1718:G:O2'   | 35:BA:1719:G:H5'  | 2.17                     | 0.44              |
| 35:BA:2203:U:H1'   | 38:BD:151:LYS:HE3 | 1.98                     | 0.44              |
| 35:BA:21:A:O2'     | 35:BA:22:C:H5'    | 2.17                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:2319:G:C2    | 35:BA:2320:A:N1    | 2.85                     | 0.44              |
| 35:BA:2712:U:H2'   | 35:BA:2713:A:H5'   | 1.99                     | 0.44              |
| 35:BA:271(H):G:H1  | 35:BA:271(P):C:N4  | 2.15                     | 0.44              |
| 35:BA:520:G:H2'    | 35:BA:521:G:H8     | 1.82                     | 0.44              |
| 35:BA:557:U:H2'    | 35:BA:558:G:H8     | 1.82                     | 0.44              |
| 35:BA:777:A:H2'    | 35:BA:778:G:H8     | 1.82                     | 0.44              |
| 35:BA:795:C:H2'    | 35:BA:796:C:C6     | 2.53                     | 0.44              |
| 35:BA:803:U:H2'    | 35:BA:804:A:C5'    | 2.48                     | 0.44              |
| 35:BA:915:C:H2'    | 35:BA:916:G:H8     | 1.83                     | 0.44              |
| 37:BC:88:GLU:N     | 37:BC:95:VAL:HG21  | 2.33                     | 0.44              |
| 38:BD:145:VAL:HG12 | 38:BD:146:GLU:O    | 2.17                     | 0.44              |
| 38:BD:177:LEU:O    | 38:BD:179:SER:N    | 2.50                     | 0.44              |
| 41:BG:97:ASP:O     | 41:BG:101:ILE:HB   | 2.17                     | 0.44              |
| 42:BH:46:GLU:CG    | 42:BH:51:ARG:HB2   | 2.46                     | 0.44              |
| 46:BN:15:LEU:C     | 46:BN:15:LEU:HD13  | 2.38                     | 0.44              |
| 48:BP:47:ASP:CB    | 48:BP:48:PRO:CA    | 2.94                     | 0.44              |
| 50:BR:11:ASN:O     | 50:BR:12:ARG:CB    | 2.64                     | 0.44              |
| 53:BU:115:ALA:C    | 53:BU:117:GLN:H    | 2.20                     | 0.44              |
| 57:BY:86:ARG:CB    | 57:BY:88:LYS:HZ1   | 2.30                     | 0.44              |
| 58:BZ:153:SER:CB   | 58:BZ:163:LEU:HD13 | 2.47                     | 0.44              |
| 1:CA:1489:G:C5     | 1:CA:1490:C:C5     | 3.06                     | 0.44              |
| 1:CA:658:G:C6      | 1:CA:749:C:N4      | 2.85                     | 0.44              |
| 1:CA:714:G:H2'     | 1:CA:715:A:C8      | 2.51                     | 0.44              |
| 1:CA:80:G:C3'      | 1:CA:81:U:H5'      | 2.35                     | 0.44              |
| 2:CB:238:LEU:O     | 2:CB:239:VAL:C     | 2.55                     | 0.44              |
| 2:CB:8:LYS:O       | 2:CB:9:GLU:C       | 2.56                     | 0.44              |
| 4:CD:8:VAL:O       | 4:CD:10:ARG:N      | 2.41                     | 0.44              |
| 5:CE:122:GLU:O     | 5:CE:123:LEU:HD23  | 2.16                     | 0.44              |
| 5:CE:139:LEU:O     | 5:CE:141:GLN:N     | 2.50                     | 0.44              |
| 7:CG:108:ALA:O     | 7:CG:111:ARG:HB2   | 2.17                     | 0.44              |
| 8:CH:17:THR:HG22   | 8:CH:63:LEU:HD12   | 1.99                     | 0.44              |
| 10:CJ:54:PHE:O     | 10:CJ:55:LYS:O     | 2.35                     | 0.44              |
| 13:CM:54:VAL:HG12  | 13:CM:58:GLU:CG    | 2.47                     | 0.44              |
| 16:CP:49:LEU:CD2   | 16:CP:73:LEU:HD22  | 2.43                     | 0.44              |
| 24:CY:25:LYS:HZ2   | 62:CY:703:GDP:PB   | 2.40                     | 0.44              |
| 24:CY:517:LEU:HB3  | 24:CY:521:SER:CB   | 2.47                     | 0.44              |
| 24:CY:519:ARG:CZ   | 24:CY:678:GLU:H    | 2.27                     | 0.44              |
| 26:D1:29:GLY:O     | 26:D1:30:VAL:HG22  | 2.18                     | 0.44              |
| 32:D7:33:ARG:HB2   | 32:D7:33:ARG:HH11  | 1.83                     | 0.44              |
| 35:DA:1019:U:N3    | 35:DA:1142(A):A:N6 | 2.66                     | 0.44              |
| 35:DA:1149:G:H2'   | 35:DA:1150:C:H6    | 1.83                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:1718:G:O2'   | 35:DA:1719:G:H5'   | 2.17                     | 0.44              |
| 35:DA:1755:A:P     | 52:DT:113:LYS:NZ   | 2.90                     | 0.44              |
| 35:DA:216:A:H2'    | 35:DA:217:G:C8     | 2.53                     | 0.44              |
| 35:DA:2292:C:O2'   | 35:DA:2293:C:H5'   | 2.17                     | 0.44              |
| 31:D6:54:ILE:HD11  | 35:DA:2420:C:H5'   | 1.98                     | 0.44              |
| 35:DA:271(K):U:H3' | 35:DA:271(L):U:C5' | 2.47                     | 0.44              |
| 35:DA:329:G:H4'    | 35:DA:330:A:OP2    | 2.17                     | 0.44              |
| 35:DA:848:G:N9     | 35:DA:933:A:H8     | 2.15                     | 0.44              |
| 38:DD:131:LEU:HD13 | 38:DD:136:ILE:HD11 | 1.99                     | 0.44              |
| 38:DD:26:LYS:O     | 38:DD:27:THR:CG2   | 2.65                     | 0.44              |
| 38:DD:94:LEU:HD23  | 38:DD:95:LEU:N     | 2.32                     | 0.44              |
| 39:DE:21:VAL:HG23  | 39:DE:21:VAL:O     | 2.16                     | 0.44              |
| 39:DE:36:ARG:CG    | 39:DE:36:ARG:NH1   | 2.77                     | 0.44              |
| 39:DE:37:ARG:HA    | 39:DE:42:ASP:OD2   | 2.16                     | 0.44              |
| 40:DF:198:ALA:C    | 40:DF:201:VAL:HG12 | 2.38                     | 0.44              |
| 40:DF:205:ARG:O    | 40:DF:206:ILE:HD13 | 2.18                     | 0.44              |
| 42:DH:86:GLU:OE2   | 42:DH:86:GLU:N     | 2.50                     | 0.44              |
| 42:DH:89:ILE:C     | 42:DH:89:ILE:HD12  | 2.38                     | 0.44              |
| 46:DN:104:LYS:HB2  | 46:DN:117:PHE:CE1  | 2.52                     | 0.44              |
| 47:DO:17:ARG:O     | 47:DO:18:LYS:HG3   | 2.17                     | 0.44              |
| 51:DS:25:ARG:CG    | 51:DS:26:LEU:H     | 2.29                     | 0.44              |
| 51:DS:58:LEU:CD1   | 51:DS:59:LYS:H     | 2.28                     | 0.44              |
| 51:DS:59:LYS:HG2   | 51:DS:60:GLY:H     | 1.79                     | 0.44              |
| 52:DT:23:ARG:HA    | 52:DT:52:ILE:HD11  | 2.00                     | 0.44              |
| 53:DU:82:GLY:C     | 53:DU:84:LYS:N     | 2.69                     | 0.44              |
| 35:DA:747:U:O2'    | 55:DW:88:ARG:HG3   | 2.17                     | 0.44              |
| 57:DY:47:LYS:HG3   | 57:DY:60:PHE:CE2   | 2.43                     | 0.44              |
| 1:AA:329:A:H3'     | 1:AA:330:C:C5'     | 2.48                     | 0.44              |
| 1:AA:417:C:H2'     | 1:AA:418:C:C6      | 2.53                     | 0.44              |
| 1:AA:451:A:O4'     | 1:AA:452:A:C8      | 2.70                     | 0.44              |
| 1:AA:841:U:H3'     | 1:AA:848:C:C5'     | 2.47                     | 0.44              |
| 2:AB:17:PHE:O      | 2:AB:18:GLY:C      | 2.55                     | 0.44              |
| 3:AC:10:PHE:CZ     | 3:AC:178:LEU:HD11  | 2.52                     | 0.44              |
| 3:AC:140:ARG:HG3   | 3:AC:140:ARG:NH1   | 2.32                     | 0.44              |
| 3:AC:131:ARG:HH22  | 3:AC:168:ALA:HB2   | 1.83                     | 0.44              |
| 4:AD:163:GLU:C     | 4:AD:165:MET:N     | 2.70                     | 0.44              |
| 10:AJ:32:ALA:CB    | 10:AJ:78:ASN:HD21  | 2.31                     | 0.44              |
| 12:AL:8:ASN:O      | 12:AL:12:ARG:HG3   | 2.18                     | 0.44              |
| 12:AL:27:LEU:C     | 12:AL:29:GLY:H     | 2.20                     | 0.44              |
| 13:AM:35:GLU:HG3   | 13:AM:36:LYS:N     | 2.32                     | 0.44              |
| 18:AR:59:SER:H     | 18:AR:62:GLU:CB    | 2.26                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 20:AT:61:SER:O    | 20:AT:63:ILE:N     | 2.50                     | 0.44              |
| 22:AV:20:U:H3'    | 22:AV:21:A:C5'     | 2.39                     | 0.44              |
| 22:AV:36:U:H1'    | 24:AY:502:GLY:HA2  | 1.99                     | 0.44              |
| 22:AV:68:C:H2'    | 22:AV:69:C:H6      | 1.81                     | 0.44              |
| 24:AY:363:ARG:CG  | 24:AY:363:ARG:HH11 | 2.25                     | 0.44              |
| 31:B6:11:LEU:HD13 | 31:B6:11:LEU:C     | 2.37                     | 0.44              |
| 31:B6:51:GLU:HG2  | 31:B6:52:VAL:N     | 2.32                     | 0.44              |
| 35:BA:1077:A:O2'  | 35:BA:1078:U:H5'   | 2.16                     | 0.44              |
| 35:BA:1654:A:O2'  | 39:BE:113:PHE:O    | 2.35                     | 0.44              |
| 35:BA:187:G:N3    | 35:BA:1365:A:H2    | 2.15                     | 0.44              |
| 35:BA:1935:G:H1'  | 35:BA:1964:G:N2    | 2.32                     | 0.44              |
| 35:BA:272(I):U:H5 | 35:BA:363(A):A:C2  | 2.35                     | 0.44              |
| 35:BA:558:G:C5'   | 46:BN:112:LEU:HD22 | 2.46                     | 0.44              |
| 35:BA:833:U:O2    | 48:BP:55:ARG:NH1   | 2.49                     | 0.44              |
| 35:BA:834:C:O2'   | 35:BA:835:A:H5'    | 2.18                     | 0.44              |
| 37:BC:156:GLU:OE1 | 37:BC:161:ARG:HD3  | 2.17                     | 0.44              |
| 37:BC:69:LEU:O    | 37:BC:70:GLY:C     | 2.55                     | 0.44              |
| 38:BD:31:LYS:O    | 38:BD:33:LEU:N     | 2.51                     | 0.44              |
| 38:BD:44:ASN:N    | 38:BD:44:ASN:OD1   | 2.49                     | 0.44              |
| 38:BD:92:ILE:CD1  | 38:BD:92:ILE:H     | 2.29                     | 0.44              |
| 39:BE:177:PRO:O   | 39:BE:178:GLU:C    | 2.56                     | 0.44              |
| 39:BE:32:PRO:CA   | 39:BE:90:THR:HG23  | 2.46                     | 0.44              |
| 40:BF:25:PRO:CB   | 40:BF:119:ARG:HB2  | 2.46                     | 0.44              |
| 41:BG:107:LEU:HA  | 41:BG:111:LEU:HD12 | 1.98                     | 0.44              |
| 42:BH:85:LYS:CD   | 42:BH:85:LYS:C     | 2.80                     | 0.44              |
| 46:BN:128:HIS:HE1 | 46:BN:134:ARG:NH1  | 2.15                     | 0.44              |
| 35:BA:2406:U:C2   | 48:BP:72:PRO:HB2   | 2.52                     | 0.44              |
| 51:BS:47:THR:CG2  | 51:BS:49:VAL:O     | 2.65                     | 0.44              |
| 53:BU:96:ALA:C    | 53:BU:98:LEU:H     | 2.20                     | 0.44              |
| 56:BX:64:LYS:NZ   | 56:BX:73:ARG:NH2   | 2.66                     | 0.44              |
| 58:BZ:101:PRO:HG2 | 58:BZ:136:PHE:HA   | 2.00                     | 0.44              |
| 58:BZ:167:PRO:O   | 58:BZ:168:GLU:CB   | 2.66                     | 0.44              |
| 58:BZ:42:VAL:CG1  | 58:BZ:43:GLU:H     | 2.23                     | 0.44              |
| 58:BZ:79:ARG:O    | 58:BZ:79:ARG:CG    | 2.65                     | 0.44              |
| 1:CA:865:A:H5'    | 1:CA:1078:U:C4     | 2.52                     | 0.44              |
| 1:CA:1244:C:O2'   | 1:CA:1245:A:H5'    | 2.17                     | 0.44              |
| 1:CA:960:U:C6     | 1:CA:1225:A:C8     | 3.05                     | 0.44              |
| 1:CA:992:U:O2'    | 1:CA:993:G:P       | 2.76                     | 0.44              |
| 2:CB:165:VAL:CG2  | 2:CB:166:ASP:H     | 2.15                     | 0.44              |
| 2:CB:169:LYS:O    | 2:CB:169:LYS:HD3   | 2.18                     | 0.44              |
| 4:CD:117:ALA:O    | 4:CD:121:VAL:HG23  | 2.18                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:CD:18:LYS:O      | 4:CD:19:LEU:HD12   | 2.17                     | 0.44              |
| 5:CE:144:THR:C     | 5:CE:146:ALA:N     | 2.71                     | 0.44              |
| 6:CF:99:ALA:O      | 6:CF:100:ASN:HB2   | 2.17                     | 0.44              |
| 7:CG:15:ASP:OD2    | 7:CG:16:LEU:N      | 2.51                     | 0.44              |
| 7:CG:79:ARG:HD2    | 7:CG:79:ARG:O      | 2.17                     | 0.44              |
| 8:CH:119:LEU:HB3   | 8:CH:123:GLU:HB3   | 2.00                     | 0.44              |
| 8:CH:40:ALA:HA     | 8:CH:45:ILE:HG13   | 1.98                     | 0.44              |
| 9:CI:125:TYR:HD2   | 9:CI:126:SER:H     | 1.66                     | 0.44              |
| 11:CK:29:ILE:HB    | 11:CK:44:SER:CB    | 2.47                     | 0.44              |
| 12:CL:47:LYS:NZ    | 12:CL:47:LYS:HB3   | 2.32                     | 0.44              |
| 12:CL:83:VAL:HG12  | 12:CL:84:LEU:N     | 2.32                     | 0.44              |
| 12:CL:86:ARG:NH2   | 12:CL:99:HIS:CG    | 2.85                     | 0.44              |
| 13:CM:35:GLU:HG3   | 13:CM:36:LYS:N     | 2.32                     | 0.44              |
| 15:CO:25:THR:O     | 15:CO:26:GLU:C     | 2.55                     | 0.44              |
| 16:CP:67:THR:HG22  | 16:CP:68:ASP:H     | 1.82                     | 0.44              |
| 17:CQ:59:ILE:HG22  | 17:CQ:71:PHE:CD1   | 2.51                     | 0.44              |
| 18:CR:69:THR:O     | 18:CR:72:ARG:HB2   | 2.18                     | 0.44              |
| 24:CY:356:LEU:HD12 | 24:CY:365:GLU:HA   | 1.99                     | 0.44              |
| 24:CY:602:LEU:N    | 24:CY:602:LEU:HD23 | 2.32                     | 0.44              |
| 28:D3:4:LEU:HD23   | 28:D3:58:VAL:HA    | 1.99                     | 0.44              |
| 29:D4:22:ILE:HG22  | 29:D4:24:THR:HG23  | 1.99                     | 0.44              |
| 29:D4:31:ILE:HG23  | 29:D4:33:VAL:HG23  | 1.99                     | 0.44              |
| 30:D5:7:PRO:HG2    | 35:DA:2016:U:O2    | 2.17                     | 0.44              |
| 35:DA:1899:G:N2    | 35:DA:1902:C:C5    | 2.85                     | 0.44              |
| 35:DA:1948:G:C5'   | 35:DA:1948:G:C8    | 2.99                     | 0.44              |
| 35:DA:2656:U:C4    | 35:DA:2665:A:H2    | 2.35                     | 0.44              |
| 35:DA:322:A:P      | 40:DF:169:ASN:HD22 | 2.40                     | 0.44              |
| 35:DA:36:G:H4'     | 35:DA:451:C:C2     | 2.53                     | 0.44              |
| 36:DB:118:G:C2     | 36:DB:119:G:N7     | 2.86                     | 0.44              |
| 36:DB:28:C:O2'     | 36:DB:29:A:H5'     | 2.17                     | 0.44              |
| 37:DC:69:LEU:O     | 37:DC:70:GLY:C     | 2.55                     | 0.44              |
| 38:DD:91:ARG:O     | 38:DD:107:ALA:HB3  | 2.17                     | 0.44              |
| 38:DD:259:THR:O    | 38:DD:260:ARG:O    | 2.36                     | 0.44              |
| 38:DD:33:LEU:C     | 38:DD:33:LEU:HD23  | 2.38                     | 0.44              |
| 38:DD:77:ALA:HA    | 38:DD:97:TYR:HA    | 1.99                     | 0.44              |
| 39:DE:51:PHE:HD1   | 39:DE:52:LEU:N     | 2.15                     | 0.44              |
| 42:DH:110:SER:O    | 42:DH:111:HIS:HB2  | 2.18                     | 0.44              |
| 44:DK:77:LEU:HD13  | 44:DK:110:GLN:OE1  | 2.17                     | 0.44              |
| 45:DL:76:UNK:C     | 45:DL:78:UNK:N     | 2.80                     | 0.44              |
| 47:DO:120:GLU:OE2  | 47:DO:122:LEU:HD21 | 2.17                     | 0.44              |
| 49:DQ:65:PHE:N     | 49:DQ:65:PHE:CD2   | 2.85                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 50:DR:9:LYS:C     | 50:DR:10:LEU:HG   | 2.37                     | 0.44              |
| 35:DA:534:U:O2'   | 53:DU:49:HIS:CD2  | 2.71                     | 0.44              |
| 53:DU:72:HIS:HE1  | 53:DU:107:ALA:HB2 | 1.81                     | 0.44              |
| 53:DU:83:LEU:HG   | 53:DU:88:ILE:HD11 | 1.99                     | 0.44              |
| 54:DV:4:ILE:HG22  | 54:DV:4:ILE:O     | 2.18                     | 0.44              |
| 54:DV:88:ARG:O    | 54:DV:90:PRO:HD3  | 2.17                     | 0.44              |
| 55:DW:18:ARG:HG2  | 55:DW:18:ARG:HH11 | 1.81                     | 0.44              |
| 56:DX:41:ASN:C    | 56:DX:43:VAL:N    | 2.67                     | 0.44              |
| 56:DX:59:VAL:HG12 | 56:DX:59:VAL:O    | 2.17                     | 0.44              |
| 58:DZ:5:LEU:HA    | 58:DZ:5:LEU:HD23  | 1.80                     | 0.44              |
| 1:AA:1003:G:N2    | 1:AA:1004:A:H1'   | 2.32                     | 0.44              |
| 1:AA:1026:G:H3'   | 1:AA:1027:C:C5'   | 2.48                     | 0.44              |
| 1:AA:399:G:H2'    | 1:AA:400:C:C6     | 2.52                     | 0.44              |
| 1:AA:61:G:H2'     | 1:AA:62:U:O4'     | 2.16                     | 0.44              |
| 1:AA:657:G:O2'    | 1:AA:658:G:H5'    | 2.18                     | 0.44              |
| 1:AA:66:G:H4'     | 1:AA:173:U:H5     | 1.80                     | 0.44              |
| 1:AA:80:G:C3'     | 1:AA:81:U:H5'     | 2.35                     | 0.44              |
| 4:AD:121:VAL:CA   | 4:AD:126:ILE:HD13 | 2.48                     | 0.44              |
| 8:AH:30:ARG:HH11  | 8:AH:30:ARG:HB2   | 1.82                     | 0.44              |
| 8:AH:63:LEU:N     | 8:AH:63:LEU:HD22  | 2.33                     | 0.44              |
| 10:AJ:81:THR:C    | 10:AJ:83:GLU:N    | 2.70                     | 0.44              |
| 13:AM:74:VAL:CA   | 13:AM:77:ASN:HD22 | 2.29                     | 0.44              |
| 13:AM:3:ARG:HH21  | 13:AM:7:VAL:HG13  | 1.82                     | 0.44              |
| 14:AN:44:LEU:C    | 14:AN:44:LEU:HD12 | 2.37                     | 0.44              |
| 22:AW:58:A:C2'    | 22:AW:59:A:H5'    | 2.48                     | 0.44              |
| 24:AY:146:LEU:O   | 24:AY:147:TRP:C   | 2.56                     | 0.44              |
| 24:AY:489:LYS:HA  | 24:AY:490:PRO:HD3 | 1.88                     | 0.44              |
| 24:AY:681:LYS:HD2 | 24:AY:681:LYS:C   | 2.38                     | 0.44              |
| 24:AY:681:LYS:HA  | 24:AY:684:GLN:HB2 | 2.00                     | 0.44              |
| 28:B3:44:ARG:O    | 28:B3:48:GLU:HG2  | 2.17                     | 0.44              |
| 29:B4:14:ILE:HD13 | 29:B4:22:ILE:C    | 2.38                     | 0.44              |
| 31:B6:24:GLU:HG3  | 31:B6:37:ARG:HH21 | 1.81                     | 0.44              |
| 33:B8:56:GLU:O    | 33:B8:58:ILE:N    | 2.50                     | 0.44              |
| 35:BA:86:C:H4'    | 35:BA:104:U:O2    | 2.18                     | 0.44              |
| 35:BA:1052:C:H3'  | 35:BA:1052:C:C6   | 2.51                     | 0.44              |
| 35:BA:1132:A:C4   | 35:BA:1133:U:C5   | 3.04                     | 0.44              |
| 28:B3:31:LEU:HD12 | 35:BA:1157:G:O2'  | 2.17                     | 0.44              |
| 35:BA:1218:C:H2'  | 35:BA:1219:G:C8   | 2.52                     | 0.44              |
| 35:BA:1386:C:H5'' | 35:BA:1396:U:H5   | 1.81                     | 0.44              |
| 35:BA:1682:G:H5'  | 35:BA:1762:A:O2'  | 2.17                     | 0.44              |
| 30:B5:19:ARG:HG3  | 35:BA:2046:G:H5'' | 2.00                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:B6:5:VAL:HB     | 35:BA:2284:C:P     | 2.57                     | 0.44              |
| 35:BA:2334:G:C2    | 51:BS:15:ARG:NH1   | 2.86                     | 0.44              |
| 35:BA:425:G:H2'    | 35:BA:426:C:H6     | 1.82                     | 0.44              |
| 35:BA:641:C:H2'    | 35:BA:642:G:O4'    | 2.17                     | 0.44              |
| 36:BB:21:G:O2'     | 36:BB:22:U:P       | 2.76                     | 0.44              |
| 37:BC:102:GLN:O    | 37:BC:105:LEU:N    | 2.50                     | 0.44              |
| 37:BC:138:LEU:O    | 37:BC:139:PRO:C    | 2.55                     | 0.44              |
| 37:BC:182:PRO:HB3  | 37:BC:184:GLU:OE2  | 2.17                     | 0.44              |
| 37:BC:65:LEU:HD21  | 37:BC:162:ILE:HD11 | 2.00                     | 0.44              |
| 38:BD:211:ARG:O    | 38:BD:215:LEU:HG   | 2.17                     | 0.44              |
| 38:BD:53:PHE:HA    | 38:BD:218:ARG:HB2  | 1.99                     | 0.44              |
| 39:BE:65:GLY:O     | 39:BE:67:PHE:N     | 2.51                     | 0.44              |
| 42:BH:38:SER:HA    | 42:BH:39:PRO:HD3   | 1.84                     | 0.44              |
| 44:BK:104:VAL:HG23 | 44:BK:127:ILE:CG2  | 2.48                     | 0.44              |
| 44:BK:3:LYS:HE3    | 44:BK:29:GLN:HB3   | 1.99                     | 0.44              |
| 46:BN:16:ILE:O     | 46:BN:54:VAL:HA    | 2.18                     | 0.44              |
| 47:BO:104:ARG:HE   | 52:BT:33:LYS:CE    | 2.22                     | 0.44              |
| 52:BT:96:ARG:HB3   | 52:BT:96:ARG:CZ    | 2.47                     | 0.44              |
| 53:BU:91:ASP:O     | 53:BU:92:ARG:HB3   | 2.17                     | 0.44              |
| 1:CA:1227:A:C2     | 13:CM:117:VAL:HG11 | 2.53                     | 0.44              |
| 1:CA:1255:G:H2'    | 1:CA:1279:A:H62    | 1.81                     | 0.44              |
| 1:CA:1305:G:H5''   | 21:CU:4:GLY:O      | 2.18                     | 0.44              |
| 1:CA:1422:G:H2'    | 1:CA:1423:G:H8     | 1.82                     | 0.44              |
| 1:CA:149:A:N3      | 1:CA:149:A:H2'     | 2.32                     | 0.44              |
| 1:CA:151:A:C2'     | 1:CA:152:A:H5'     | 2.48                     | 0.44              |
| 1:CA:189:G:H2'     | 1:CA:189(A):C:H6   | 1.81                     | 0.44              |
| 1:CA:414:A:O2'     | 1:CA:415:A:H5'     | 2.17                     | 0.44              |
| 1:CA:646:U:H2'     | 1:CA:647:C:C6      | 2.53                     | 0.44              |
| 3:CC:60:ALA:O      | 3:CC:61:ALA:HB2    | 2.18                     | 0.44              |
| 3:CC:82:GLU:N      | 3:CC:82:GLU:CD     | 2.70                     | 0.44              |
| 10:CJ:16:LEU:HD12  | 10:CJ:70:ARG:HD2   | 2.00                     | 0.44              |
| 15:CO:64:ARG:HB2   | 15:CO:64:ARG:CZ    | 2.48                     | 0.44              |
| 19:CS:72:GLY:C     | 19:CS:74:PHE:N     | 2.71                     | 0.44              |
| 22:CW:57:C:OP1     | 22:CW:57:C:H6      | 2.00                     | 0.44              |
| 23:CX:12:A:C3'     | 23:CX:12:A:N3      | 2.75                     | 0.44              |
| 24:CY:170:ARG:NH1  | 24:CY:205:TYR:OH   | 2.50                     | 0.44              |
| 24:CY:583:LYS:HD3  | 24:CY:583:LYS:C    | 2.37                     | 0.44              |
| 26:D1:76:ARG:HH12  | 26:D1:95:LEU:CD2   | 2.15                     | 0.44              |
| 28:D3:35:ARG:HD3   | 28:D3:37:LEU:HD21  | 1.99                     | 0.44              |
| 33:D8:56:GLU:O     | 33:D8:58:ILE:N     | 2.50                     | 0.44              |
| 35:DA:1709:U:H3    | 35:DA:1749:A:H61   | 1.65                     | 0.44              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:2131:G:C8    | 35:DA:2133:G:N3    | 2.86                     | 0.44              |
| 35:DA:2319:G:C2    | 35:DA:2320:A:N1    | 2.85                     | 0.44              |
| 35:DA:2557:G:H2'   | 35:DA:2558:C:C6    | 2.51                     | 0.44              |
| 35:DA:2762:G:H2'   | 35:DA:2763:G:H5'   | 1.98                     | 0.44              |
| 35:DA:2887:U:H2'   | 35:DA:2888:C:C6    | 2.53                     | 0.44              |
| 35:DA:979:G:N2     | 35:DA:985:C:N4     | 2.65                     | 0.44              |
| 37:DC:135:ARG:C    | 37:DC:137:LEU:H    | 2.20                     | 0.44              |
| 38:DD:5:LYS:HD2    | 38:DD:17:THR:HG22  | 1.98                     | 0.44              |
| 38:DD:239:ARG:HH21 | 38:DD:239:ARG:HG2  | 1.82                     | 0.44              |
| 38:DD:73:VAL:O     | 38:DD:75:ILE:N     | 2.50                     | 0.44              |
| 38:DD:77:ALA:O     | 38:DD:116:GLN:HG3  | 2.18                     | 0.44              |
| 39:DE:50:GLY:HA3   | 39:DE:74:PRO:HG3   | 1.99                     | 0.44              |
| 41:DG:38:VAL:HG12  | 41:DG:93:THR:HA    | 2.00                     | 0.44              |
| 43:DJ:55:UNK:O     | 43:DJ:56:UNK:C     | 2.65                     | 0.44              |
| 47:DO:14:THR:O     | 47:DO:14:THR:HG22  | 2.17                     | 0.44              |
| 48:DP:31:ALA:C     | 48:DP:33:ARG:N     | 2.70                     | 0.44              |
| 49:DQ:110:THR:HG23 | 49:DQ:113:GLN:HG3  | 1.99                     | 0.44              |
| 49:DQ:35:VAL:CG2   | 49:DQ:36:ALA:N     | 2.81                     | 0.44              |
| 50:DR:2:ARG:HB2    | 50:DR:5:LYS:HZ3    | 1.83                     | 0.44              |
| 54:DV:40:LEU:N     | 54:DV:40:LEU:CD2   | 2.80                     | 0.44              |
| 49:DQ:62:GLY:CA    | 58:DZ:116:VAL:HG21 | 2.45                     | 0.44              |
| 58:DZ:12:GLY:CA    | 58:DZ:36:LYS:HZ3   | 2.29                     | 0.44              |
| 1:AA:1074:G:O2'    | 1:AA:1075:C:H5'    | 2.17                     | 0.44              |
| 1:AA:1430:C:H2'    | 1:AA:1431:C:C6     | 2.53                     | 0.44              |
| 1:AA:197:A:H4'     | 1:AA:198:G:H5'     | 1.98                     | 0.44              |
| 1:AA:421:U:H2'     | 1:AA:421:U:O2      | 2.17                     | 0.44              |
| 1:AA:833:U:H2'     | 1:AA:834:C:H6      | 1.80                     | 0.44              |
| 2:AB:144:ARG:O     | 2:AB:145:LEU:C     | 2.56                     | 0.44              |
| 2:AB:213:LEU:HD23  | 2:AB:213:LEU:O     | 2.18                     | 0.44              |
| 3:AC:90:GLU:OE1    | 3:AC:93:LYS:HD2    | 2.17                     | 0.44              |
| 4:AD:110:PHE:N     | 4:AD:110:PHE:CD1   | 2.85                     | 0.44              |
| 5:AE:33:VAL:CG1    | 5:AE:34:VAL:N      | 2.80                     | 0.44              |
| 7:AG:21:VAL:HG23   | 7:AG:22:LEU:N      | 2.32                     | 0.44              |
| 8:AH:34:GLU:O      | 8:AH:35:ILE:C      | 2.54                     | 0.44              |
| 8:AH:6:ILE:N       | 8:AH:6:ILE:CD1     | 2.79                     | 0.44              |
| 9:AI:125:TYR:CD2   | 9:AI:126:SER:N     | 2.85                     | 0.44              |
| 12:AL:7:ILE:HG22   | 12:AL:8:ASN:N      | 2.32                     | 0.44              |
| 12:AL:86:ARG:HH22  | 12:AL:99:HIS:CD2   | 2.35                     | 0.44              |
| 15:AO:64:ARG:CZ    | 15:AO:64:ARG:HB2   | 2.47                     | 0.44              |
| 19:AS:58:VAL:O     | 19:AS:58:VAL:CG2   | 2.65                     | 0.44              |
| 21:AU:24:ARG:HG2   | 21:AU:24:ARG:HH11  | 1.82                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 22:AV:54:5MU:C2'    | 22:AV:55:U:H5'    | 2.47                     | 0.44              |
| 24:AY:486:THR:HG22  | 24:AY:602:LEU:HG  | 1.99                     | 0.44              |
| 24:AY:529:ILE:HD11  | 24:AY:567:LEU:CD1 | 2.48                     | 0.44              |
| 24:AY:409:ILE:HD12  | 24:AY:654:GLY:HA2 | 1.97                     | 0.44              |
| 25:B0:34:GLY:O      | 25:B0:35:ASN:C    | 2.55                     | 0.44              |
| 25:B0:60:PHE:HE2    | 35:BA:2365:G:C4'  | 2.27                     | 0.44              |
| 27:B2:2:LYS:HE3     | 27:B2:52:ASP:OD1  | 2.18                     | 0.44              |
| 29:B4:35:VAL:HG12   | 29:B4:36:CYS:N    | 2.32                     | 0.44              |
| 30:B5:44:THR:CG2    | 30:B5:45:VAL:H    | 2.22                     | 0.44              |
| 31:B6:5:VAL:CG2     | 35:BA:2283:C:OP1  | 2.65                     | 0.44              |
| 32:B7:5:TRP:CZ3     | 35:BA:464:U:H4'   | 2.53                     | 0.44              |
| 33:B8:32:LEU:O      | 33:B8:33:ASN:O    | 2.35                     | 0.44              |
| 35:BA:1213:A:N3     | 35:BA:1238:G:H1'  | 2.32                     | 0.44              |
| 35:BA:1445(A):C:H5' | 35:BA:1446:C:OP2  | 2.17                     | 0.44              |
| 35:BA:1408:C:H42    | 35:BA:1594:G:H1   | 1.66                     | 0.44              |
| 35:BA:191:A:O2'     | 35:BA:192:C:H5'   | 2.17                     | 0.44              |
| 35:BA:1971:A:N3     | 38:BD:240:ALA:HA  | 2.33                     | 0.44              |
| 35:BA:205:G:O2'     | 35:BA:206:U:P     | 2.76                     | 0.44              |
| 35:BA:198:C:N4      | 35:BA:248:G:H1    | 2.14                     | 0.44              |
| 35:BA:2543:G:C2     | 35:BA:2765:A:H2'  | 2.52                     | 0.44              |
| 35:BA:2550:G:C6     | 35:BA:2551:C:N4   | 2.86                     | 0.44              |
| 35:BA:484:C:H2'     | 35:BA:485:C:C6    | 2.52                     | 0.44              |
| 35:BA:637:A:OP1     | 48:BP:133:SER:CB  | 2.66                     | 0.44              |
| 35:BA:777:A:H2'     | 35:BA:778:G:C8    | 2.52                     | 0.44              |
| 35:BA:841:A:H2'     | 35:BA:842:G:O4'   | 2.17                     | 0.44              |
| 35:BA:892:G:O2'     | 35:BA:893:C:H5'   | 2.18                     | 0.44              |
| 35:BA:914:C:C2'     | 35:BA:915:C:H5'   | 2.42                     | 0.44              |
| 35:BA:848:G:N9      | 35:BA:933:A:H8    | 2.15                     | 0.44              |
| 37:BC:115:VAL:HA    | 37:BC:145:THR:CG2 | 2.46                     | 0.44              |
| 37:BC:211:ARG:HG3   | 37:BC:211:ARG:NH1 | 2.32                     | 0.44              |
| 38:BD:70:TRP:HH2    | 38:BD:150:LYS:HA  | 1.76                     | 0.44              |
| 35:BA:1820:U:C2     | 38:BD:202:LYS:HG2 | 2.53                     | 0.44              |
| 39:BE:51:PHE:HD1    | 39:BE:52:LEU:HD12 | 1.82                     | 0.44              |
| 41:BG:97:ASP:CB     | 41:BG:98:ARG:HH12 | 2.19                     | 0.44              |
| 46:BN:119:ARG:NH1   | 46:BN:119:ARG:HG3 | 2.33                     | 0.44              |
| 46:BN:57:ALA:O      | 46:BN:58:ASP:C    | 2.55                     | 0.44              |
| 47:BO:52:VAL:C      | 47:BO:53:LYS:HG3  | 2.37                     | 0.44              |
| 50:BR:118:GLU:HA    | 50:BR:118:GLU:OE1 | 2.18                     | 0.44              |
| 50:BR:33:ARG:HG3    | 50:BR:115:GLU:HG3 | 2.00                     | 0.44              |
| 52:BT:28:VAL:O      | 52:BT:28:VAL:HG12 | 2.17                     | 0.44              |
| 47:BO:104:ARG:NH2   | 52:BT:33:LYS:CE   | 2.80                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:BT:57:PHE:CG    | 52:BT:58:ASN:N     | 2.82                     | 0.44              |
| 53:BU:115:ALA:C    | 53:BU:117:GLN:N    | 2.70                     | 0.44              |
| 53:BU:92:ARG:HB3   | 54:BV:11:GLN:NE2   | 2.33                     | 0.44              |
| 55:BW:47:VAL:O     | 55:BW:47:VAL:CG1   | 2.66                     | 0.44              |
| 56:BX:59:VAL:O     | 56:BX:59:VAL:HG12  | 2.16                     | 0.44              |
| 1:CA:1065:U:O2'    | 1:CA:1066:C:P      | 2.76                     | 0.44              |
| 1:CA:1347:G:H2'    | 1:CA:1373:G:C6     | 2.52                     | 0.44              |
| 1:CA:37:U:O2'      | 1:CA:500:G:H4'     | 2.17                     | 0.44              |
| 8:CH:35:ILE:HG23   | 8:CH:111:ILE:HD13  | 2.00                     | 0.44              |
| 13:CM:66:LEU:N     | 13:CM:66:LEU:CD1   | 2.72                     | 0.44              |
| 20:CT:42:GLN:CA    | 20:CT:42:GLN:NE2   | 2.78                     | 0.44              |
| 20:CT:75:ASN:HD22  | 20:CT:75:ASN:H     | 1.65                     | 0.44              |
| 22:CV:4:G:HO2'     | 22:CV:5:G:H8       | 1.63                     | 0.44              |
| 23:CX:17:U:O2'     | 23:CX:18:G:H5'     | 2.18                     | 0.44              |
| 24:CY:447:GLY:O    | 24:CY:449:THR:N    | 2.51                     | 0.44              |
| 24:CY:617:MET:HE3  | 24:CY:641:GLN:CB   | 2.48                     | 0.44              |
| 24:CY:616:TYR:HB3  | 24:CY:662:LYS:O    | 2.17                     | 0.44              |
| 24:CY:71:THR:HB    | 24:CY:78:ARG:HH12  | 1.82                     | 0.44              |
| 31:D6:11:LEU:CB    | 31:D6:26:ASN:HD21  | 2.31                     | 0.44              |
| 33:D8:4:MET:O      | 33:D8:62:LEU:CD1   | 2.65                     | 0.44              |
| 33:D8:56:GLU:C     | 33:D8:58:ILE:N     | 2.71                     | 0.44              |
| 27:D2:69:ARG:HH22  | 35:DA:111:A:H4'    | 1.83                     | 0.44              |
| 35:DA:1782:C:H1'   | 35:DA:2609:U:C5'   | 2.38                     | 0.44              |
| 35:DA:2288:A:C2    | 35:DA:2325:G:N7    | 2.86                     | 0.44              |
| 35:DA:2722:G:O2'   | 50:DR:5:LYS:HB2    | 2.18                     | 0.44              |
| 35:DA:2779:U:H5'   | 35:DA:2780:G:O5'   | 2.17                     | 0.44              |
| 35:DA:460:A:C2     | 35:DA:470:A:C4     | 3.05                     | 0.44              |
| 25:D0:26:TYR:CE2   | 35:DA:857:C:H1'    | 2.48                     | 0.44              |
| 35:DA:943:U:OP2    | 48:DP:38:GLN:OE1   | 2.36                     | 0.44              |
| 36:DB:9:G:C6       | 36:DB:113:G:C6     | 3.06                     | 0.44              |
| 36:DB:29:A:OP2     | 51:DS:32:LEU:HG    | 2.18                     | 0.44              |
| 37:DC:115:VAL:HG12 | 37:DC:145:THR:CG2  | 2.46                     | 0.44              |
| 39:DE:96:PHE:HA    | 39:DE:100:GLU:OE1  | 2.17                     | 0.44              |
| 39:DE:132:HIS:CG   | 39:DE:135:HIS:NE2  | 2.85                     | 0.44              |
| 39:DE:23:VAL:CG1   | 39:DE:173:VAL:HG21 | 2.47                     | 0.44              |
| 39:DE:9:VAL:HG22   | 39:DE:10:GLY:H     | 1.81                     | 0.44              |
| 41:DG:110:ALA:O    | 41:DG:111:LEU:C    | 2.55                     | 0.44              |
| 41:DG:55:LYS:HD3   | 41:DG:55:LYS:C     | 2.36                     | 0.44              |
| 41:DG:60:LEU:O     | 41:DG:64:THR:HG22  | 2.17                     | 0.44              |
| 44:DK:105:LEU:CD2  | 44:DK:120:LEU:HD13 | 2.47                     | 0.44              |
| 44:DK:30:HIS:CA    | 44:DK:59:ILE:HD12  | 2.39                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 46:DN:120:LEU:HD13 | 46:DN:120:LEU:C     | 2.38                     | 0.44              |
| 46:DN:32:THR:HG23  | 46:DN:37:LYS:HB3    | 1.99                     | 0.44              |
| 47:DO:37:ASP:O     | 47:DO:62:VAL:HG23   | 2.17                     | 0.44              |
| 35:DA:662:G:P      | 48:DP:18:ARG:HD2    | 2.57                     | 0.44              |
| 50:DR:48:VAL:HG12  | 50:DR:52:ILE:HG12   | 1.99                     | 0.44              |
| 51:DS:12:PHE:C     | 51:DS:12:PHE:HD1    | 2.21                     | 0.44              |
| 52:DT:107:ASP:CG   | 52:DT:108:ARG:N     | 2.67                     | 0.44              |
| 52:DT:117:ASP:O    | 52:DT:118:ARG:C     | 2.56                     | 0.44              |
| 57:DY:105:ALA:C    | 57:DY:107:ASP:N     | 2.71                     | 0.44              |
| 1:AA:1327:C:OP2    | 21:AU:12:LYS:NZ     | 2.49                     | 0.44              |
| 1:AA:189:G:H2'     | 1:AA:189(A):C:H6    | 1.81                     | 0.44              |
| 1:AA:321:A:C2      | 1:AA:333:G:C2       | 3.06                     | 0.44              |
| 1:AA:346:G:P       | 52:BT:41:ARG:NH2    | 2.90                     | 0.44              |
| 1:AA:357:G:O2'     | 1:AA:358:U:H5'      | 2.17                     | 0.44              |
| 1:AA:373:A:H2'     | 1:AA:374:A:H8       | 1.81                     | 0.44              |
| 1:AA:659:U:O2'     | 1:AA:660:G:H5'      | 2.18                     | 0.44              |
| 3:AC:111:LEU:CD2   | 3:AC:141:VAL:HG13   | 2.48                     | 0.44              |
| 5:AE:33:VAL:HG12   | 5:AE:112:LEU:HD12   | 2.00                     | 0.44              |
| 8:AH:35:ILE:HG23   | 8:AH:111:ILE:HD13   | 2.00                     | 0.44              |
| 8:AH:85:ARG:HH12   | 8:AH:134:ILE:HG23   | 1.82                     | 0.44              |
| 13:AM:46:LYS:HD3   | 13:AM:46:LYS:O      | 2.17                     | 0.44              |
| 15:AO:18:PHE:CD1   | 15:AO:18:PHE:O      | 2.71                     | 0.44              |
| 16:AP:15:PRO:O     | 16:AP:16:HIS:ND1    | 2.51                     | 0.44              |
| 17:AQ:43:LEU:HD23  | 17:AQ:43:LEU:HA     | 1.74                     | 0.44              |
| 24:AY:196:ILE:CG1  | 24:AY:197:ARG:N     | 2.78                     | 0.44              |
| 24:AY:227:ILE:O    | 24:AY:227:ILE:CG2   | 2.66                     | 0.44              |
| 24:AY:297:GLU:HG3  | 24:AY:297:GLU:O     | 2.16                     | 0.44              |
| 24:AY:524:GLU:O    | 24:AY:565:VAL:N     | 2.32                     | 0.44              |
| 24:AY:539:ILE:CD1  | 24:AY:567:LEU:HD21  | 2.48                     | 0.44              |
| 26:B1:56:GLN:CA    | 26:B1:56:GLN:HE21   | 2.15                     | 0.44              |
| 29:B4:5:ILE:HD13   | 29:B4:6:HIS:CD2     | 2.53                     | 0.44              |
| 35:BA:1185:C:C5'   | 35:BA:1186:G:P      | 3.06                     | 0.44              |
| 35:BA:1445(A):C:O2 | 35:BA:1445(A):C:H2' | 2.16                     | 0.44              |
| 35:BA:214:G:H1'    | 35:BA:216:A:HO2'    | 1.81                     | 0.44              |
| 35:BA:2543:G:H2'   | 35:BA:2544:G:C8     | 2.52                     | 0.44              |
| 35:BA:301:G:HO2'   | 35:BA:302:C:H6      | 1.63                     | 0.44              |
| 35:BA:527:C:O2     | 35:BA:527:C:O4'     | 2.35                     | 0.44              |
| 35:BA:63:U:H4'     | 35:BA:63:U:OP1      | 2.17                     | 0.44              |
| 36:BB:118:G:C2     | 36:BB:119:G:N7      | 2.86                     | 0.44              |
| 38:BD:81:ALA:HA    | 38:BD:113:VAL:HG22  | 1.99                     | 0.44              |
| 42:BH:103:LEU:HB2  | 42:BH:123:PHE:CD2   | 2.53                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 46:BN:43:THR:HG22  | 46:BN:45:ASN:ND2    | 2.33                     | 0.44              |
| 49:BQ:52:VAL:C     | 49:BQ:54:MET:N      | 2.71                     | 0.44              |
| 49:BQ:75:THR:HG22  | 49:BQ:76:LYS:H      | 1.82                     | 0.44              |
| 50:BR:18:LEU:HD21  | 50:BR:22:ARG:CZ     | 2.48                     | 0.44              |
| 50:BR:92:GLY:HA2   | 50:BR:94:TYR:CE1    | 2.53                     | 0.44              |
| 52:BT:113:LYS:C    | 52:BT:114:LEU:HD23  | 2.38                     | 0.44              |
| 52:BT:49:VAL:O     | 52:BT:49:VAL:HG22   | 2.17                     | 0.44              |
| 35:BA:997:G:OP1    | 53:BU:93:LYS:HD3    | 2.17                     | 0.44              |
| 54:BV:28:GLU:CB    | 54:BV:31:ALA:HB2    | 2.36                     | 0.44              |
| 58:BZ:41:LEU:HD23  | 58:BZ:41:LEU:HA     | 1.73                     | 0.44              |
| 1:CA:1080:A:H5''   | 5:CE:16:THR:HG21    | 1.99                     | 0.44              |
| 1:CA:1371:G:C6     | 1:CA:1372:U:C4      | 3.06                     | 0.44              |
| 1:CA:923:A:O4'     | 1:CA:1398:A:C2      | 2.70                     | 0.44              |
| 1:CA:1418:A:H3'    | 1:CA:1419:G:O4'     | 2.17                     | 0.44              |
| 1:CA:421:U:O2      | 1:CA:421:U:H2'      | 2.17                     | 0.44              |
| 1:CA:781:A:C3'     | 1:CA:782:A:H5'      | 2.48                     | 0.44              |
| 1:CA:930:C:O2'     | 1:CA:931:C:H5'      | 2.18                     | 0.44              |
| 1:CA:957:U:O2      | 1:CA:959:A:H8       | 2.01                     | 0.44              |
| 3:CC:43:LEU:O      | 3:CC:45:LYS:N       | 2.50                     | 0.44              |
| 4:CD:30:LYS:HB3    | 4:CD:35:ARG:HD2     | 1.99                     | 0.44              |
| 5:CE:9:LYS:NZ      | 5:CE:111:GLU:OE1    | 2.51                     | 0.44              |
| 8:CH:74:PRO:O      | 8:CH:75:ARG:C       | 2.56                     | 0.44              |
| 10:CJ:27:ALA:HA    | 10:CJ:30:SER:OG     | 2.18                     | 0.44              |
| 11:CK:120:ARG:HA   | 11:CK:121:PRO:HD3   | 1.84                     | 0.44              |
| 11:CK:87:THR:O     | 11:CK:88:GLY:C      | 2.54                     | 0.44              |
| 18:CR:71:LYS:O     | 18:CR:74:ARG:HB2    | 2.16                     | 0.44              |
| 21:CU:2:GLY:C      | 21:CU:4:GLY:H       | 2.21                     | 0.44              |
| 22:CW:68:C:H2'     | 22:CW:69:C:C5       | 2.52                     | 0.44              |
| 24:CY:230:LYS:NZ   | 24:CY:237:PRO:CA    | 2.76                     | 0.44              |
| 25:D0:78:TYR:H     | 25:D0:78:TYR:HD1    | 1.65                     | 0.44              |
| 27:D2:13:ALA:HA    | 27:D2:16:LEU:HD12   | 1.98                     | 0.44              |
| 31:D6:12:GLU:HA    | 31:D6:23:THR:HA     | 1.99                     | 0.44              |
| 35:DA:1011:G:O2'   | 35:DA:1013:C:H5''   | 2.17                     | 0.44              |
| 35:DA:2174:C:O2'   | 35:DA:2175:C:H5'    | 2.17                     | 0.44              |
| 35:DA:2352:A:H2'   | 35:DA:2353:G:H5'    | 2.00                     | 0.44              |
| 35:DA:2577:A:C5'   | 35:DA:2578:G:C5'    | 2.96                     | 0.44              |
| 35:DA:271(M):G:H2' | 35:DA:271(N):U:H5'' | 1.99                     | 0.44              |
| 35:DA:2778:A:C5'   | 35:DA:2779:U:OP2    | 2.59                     | 0.44              |
| 35:DA:2840:C:H2'   | 35:DA:2841:C:C6     | 2.53                     | 0.44              |
| 35:DA:41:C:N4      | 35:DA:437:G:H1      | 2.15                     | 0.44              |
| 36:DB:67:G:O2'     | 36:DB:68:C:H5'      | 2.18                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:DD:81:ALA:HA    | 38:DD:113:VAL:HG22 | 1.99                     | 0.44              |
| 39:DE:119:ARG:NH1  | 39:DE:156:MET:O    | 2.51                     | 0.44              |
| 39:DE:25:VAL:HG22  | 39:DE:183:LEU:HG   | 2.00                     | 0.44              |
| 39:DE:93:VAL:HG12  | 39:DE:175:VAL:CG2  | 2.47                     | 0.44              |
| 41:DG:153:ARG:HB3  | 41:DG:153:ARG:HH11 | 1.83                     | 0.44              |
| 41:DG:37:VAL:CG2   | 41:DG:159:VAL:HA   | 2.48                     | 0.44              |
| 44:DK:104:VAL:HG23 | 44:DK:127:ILE:CG2  | 2.48                     | 0.44              |
| 49:DQ:17:LEU:O     | 49:DQ:18:LYS:HD2   | 2.17                     | 0.44              |
| 50:DR:12:ARG:HD3   | 50:DR:16:HIS:CD2   | 2.53                     | 0.44              |
| 52:DT:23:ARG:C     | 52:DT:25:GLY:H     | 2.13                     | 0.44              |
| 53:DU:112:ARG:HG2  | 53:DU:112:ARG:HH11 | 1.82                     | 0.44              |
| 53:DU:55:ARG:HA    | 53:DU:58:ARG:CB    | 2.47                     | 0.44              |
| 57:DY:10:GLY:C     | 57:DY:27:VAL:HG22  | 2.37                     | 0.44              |
| 57:DY:31:LEU:CD2   | 57:DY:31:LEU:N     | 2.78                     | 0.44              |
| 58:DZ:144:LEU:HD22 | 58:DZ:144:LEU:N    | 2.33                     | 0.44              |
| 58:DZ:69:THR:HG22  | 58:DZ:90:VAL:CA    | 2.20                     | 0.44              |
| 1:AA:1296:C:H3'    | 1:AA:1297:C:H6     | 1.83                     | 0.44              |
| 1:AA:1308:U:C5     | 13:AM:99:ARG:NH1   | 2.85                     | 0.44              |
| 1:AA:154:C:H2'     | 1:AA:155:C:C6      | 2.53                     | 0.44              |
| 1:AA:220:G:N2      | 1:AA:221:C:H1'     | 2.33                     | 0.44              |
| 1:AA:40:C:H2'      | 1:AA:41:G:H8       | 1.82                     | 0.44              |
| 1:AA:994:A:H2'     | 1:AA:994:A:N3      | 2.32                     | 0.44              |
| 2:AB:137:ARG:HG2   | 2:AB:137:ARG:NH1   | 2.33                     | 0.44              |
| 3:AC:60:ALA:N      | 3:AC:63:ASN:OD1    | 2.51                     | 0.44              |
| 5:AE:6:PHE:CD1     | 5:AE:6:PHE:N       | 2.85                     | 0.44              |
| 7:AG:102:ARG:HG2   | 7:AG:106:GLN:HE21  | 1.81                     | 0.44              |
| 1:AA:1298:C:H5''   | 7:AG:114:ARG:NH2   | 2.31                     | 0.44              |
| 1:AA:1375:A:OP1    | 7:AG:12:LEU:HD21   | 2.18                     | 0.44              |
| 7:AG:57:GLU:O      | 7:AG:58:PRO:C      | 2.56                     | 0.44              |
| 8:AH:30:ARG:HB3    | 8:AH:30:ARG:NH1    | 2.32                     | 0.44              |
| 12:AL:110:VAL:CG2  | 12:AL:120:TYR:HB3  | 2.48                     | 0.44              |
| 13:AM:35:GLU:CG    | 13:AM:36:LYS:N     | 2.80                     | 0.44              |
| 13:AM:54:VAL:C     | 13:AM:56:LEU:N     | 2.71                     | 0.44              |
| 18:AR:58:LEU:CD1   | 18:AR:58:LEU:N     | 2.80                     | 0.44              |
| 24:AY:162:VAL:HG23 | 24:AY:255:ILE:HG13 | 1.99                     | 0.44              |
| 24:AY:369:LEU:N    | 24:AY:369:LEU:HD12 | 2.33                     | 0.44              |
| 24:AY:486:THR:O    | 24:AY:599:PRO:HA   | 2.17                     | 0.44              |
| 24:AY:519:ARG:CZ   | 24:AY:678:GLU:H    | 2.30                     | 0.44              |
| 35:BA:1034:G:H8    | 35:BA:1034:G:OP1   | 1.99                     | 0.44              |
| 35:BA:1472:A:H2'   | 35:BA:1473:G:H8    | 1.81                     | 0.44              |
| 35:BA:1551:C:H2'   | 35:BA:1552:G:O4'   | 2.18                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:1632:A:C5    | 35:BA:1633:G:C6    | 3.05                     | 0.44              |
| 35:BA:1722:A:C2    | 35:BA:1740:G:C8    | 3.06                     | 0.44              |
| 35:BA:2088:G:C6    | 35:BA:2089:U:C4    | 3.05                     | 0.44              |
| 35:BA:2656:U:C4    | 35:BA:2665:A:H2    | 2.35                     | 0.44              |
| 35:BA:2689:U:H4'   | 35:BA:2690:C:OP2   | 2.17                     | 0.44              |
| 35:BA:863:A:O2'    | 36:BB:101:G:H1'    | 2.18                     | 0.44              |
| 35:BA:930:U:H4'    | 35:BA:931:G:O5'    | 2.18                     | 0.44              |
| 37:BC:16:ASP:O     | 37:BC:18:ASN:N     | 2.50                     | 0.44              |
| 40:BF:132:VAL:O    | 40:BF:133:ASN:HB2  | 2.18                     | 0.44              |
| 40:BF:198:ALA:C    | 40:BF:201:VAL:HG12 | 2.38                     | 0.44              |
| 29:B4:1:MET:SD     | 41:BG:98:ARG:HG3   | 2.58                     | 0.44              |
| 42:BH:141:VAL:O    | 42:BH:142:GLY:C    | 2.56                     | 0.44              |
| 42:BH:169:VAL:CG2  | 42:BH:170:ARG:N    | 2.78                     | 0.44              |
| 42:BH:94:TYR:CD2   | 42:BH:107:VAL:HG12 | 2.53                     | 0.44              |
| 46:BN:60:ILE:HG22  | 46:BN:61:ARG:N     | 2.33                     | 0.44              |
| 49:BQ:137:TYR:CD1  | 49:BQ:137:TYR:N    | 2.85                     | 0.44              |
| 50:BR:21:TYR:OH    | 50:BR:43:GLU:HG2   | 2.16                     | 0.44              |
| 51:BS:56:LEU:O     | 51:BS:58:LEU:N     | 2.51                     | 0.44              |
| 52:BT:116:ALA:HB1  | 52:BT:121:ILE:HD11 | 1.99                     | 0.44              |
| 52:BT:50:ILE:N     | 52:BT:50:ILE:CD1   | 2.80                     | 0.44              |
| 53:BU:112:ARG:HG2  | 53:BU:112:ARG:HH11 | 1.83                     | 0.44              |
| 58:BZ:115:GLY:HA2  | 58:BZ:177:PRO:HD3  | 1.99                     | 0.44              |
| 58:BZ:141:VAL:HG13 | 58:BZ:144:LEU:HD23 | 1.99                     | 0.44              |
| 58:BZ:9:TYR:CE1    | 58:BZ:35:ARG:NH1   | 2.79                     | 0.44              |
| 1:CA:10:A:H2'      | 1:CA:11:G:C8       | 2.52                     | 0.44              |
| 1:CA:1118:C:OP1    | 9:CI:104:ARG:NH1   | 2.51                     | 0.44              |
| 1:CA:1388:C:H2'    | 1:CA:1389:C:C6     | 2.52                     | 0.44              |
| 1:CA:271:C:H2'     | 1:CA:272:C:H6      | 1.82                     | 0.44              |
| 1:CA:356:A:H1'     | 1:CA:368:U:O2'     | 2.18                     | 0.44              |
| 1:CA:541:G:O2'     | 1:CA:542:G:H5'     | 2.17                     | 0.44              |
| 1:CA:747:C:H2'     | 1:CA:748:C:C1'     | 2.48                     | 0.44              |
| 1:CA:909:A:H2'     | 1:CA:910:C:O4'     | 2.18                     | 0.44              |
| 1:CA:1343:G:H1'    | 9:CI:121:ARG:HH12  | 1.83                     | 0.44              |
| 9:CI:82:ALA:HA     | 9:CI:85:LEU:CD1    | 2.48                     | 0.44              |
| 12:CL:6:THR:H      | 12:CL:9:GLN:HE21   | 1.65                     | 0.44              |
| 18:CR:66:LEU:CG    | 18:CR:70:ILE:HD11  | 2.47                     | 0.44              |
| 18:CR:79:LEU:HD22  | 18:CR:80:PRO:HD2   | 2.00                     | 0.44              |
| 20:CT:104:LEU:HD23 | 20:CT:105:SER:O    | 2.17                     | 0.44              |
| 24:CY:223:PHE:HB3  | 24:CY:248:LYS:HD3  | 1.98                     | 0.44              |
| 24:CY:327:PHE:HA   | 24:CY:376:ALA:HA   | 2.00                     | 0.44              |
| 24:CY:489:LYS:HA   | 24:CY:490:PRO:HD3  | 1.71                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:CY:644:ARG:O    | 24:CY:645:ALA:HB2  | 2.17                     | 0.44              |
| 34:D9:4:ARG:NH1    | 35:DA:2477:C:N4    | 2.66                     | 0.44              |
| 35:DA:1331:A:O2'   | 35:DA:1332:G:H8    | 2.01                     | 0.44              |
| 35:DA:1381:G:N2    | 35:DA:1382:G:H1'   | 2.32                     | 0.44              |
| 35:DA:1343:G:N3    | 35:DA:1384:A:H2    | 2.16                     | 0.44              |
| 35:DA:2032:G:OP2   | 35:DA:2454:G:O2'   | 2.30                     | 0.44              |
| 35:DA:2681:C:H5    | 35:DA:2725:A:N6    | 2.14                     | 0.44              |
| 35:DA:2849:U:O4    | 52:DT:23:ARG:NH2   | 2.51                     | 0.44              |
| 35:DA:294:A:H2'    | 35:DA:295:G:H5'    | 1.99                     | 0.44              |
| 35:DA:458:G:N2     | 35:DA:469:G:H2'    | 2.33                     | 0.44              |
| 35:DA:483:A:C2     | 35:DA:484:C:H1'    | 2.52                     | 0.44              |
| 35:DA:484:C:H2'    | 35:DA:485:C:C6     | 2.52                     | 0.44              |
| 35:DA:783:A:H2'    | 35:DA:784:A:O5'    | 2.18                     | 0.44              |
| 37:DC:148:PHE:C    | 37:DC:150:ILE:H    | 2.21                     | 0.44              |
| 35:DA:2122:U:H4'   | 37:DC:167:ASP:HB3  | 2.00                     | 0.44              |
| 37:DC:78:ILE:HG21  | 37:DC:124:VAL:CG2  | 2.47                     | 0.44              |
| 38:DD:146:GLU:HG2  | 38:DD:152:GLY:O    | 2.18                     | 0.44              |
| 38:DD:165:ILE:HD13 | 38:DD:175:LEU:HD21 | 1.98                     | 0.44              |
| 38:DD:48:ARG:NH1   | 38:DD:48:ARG:HG3   | 2.33                     | 0.44              |
| 40:DF:116:ASP:OD2  | 48:DP:5:ASP:HB2    | 2.18                     | 0.44              |
| 40:DF:119:ARG:NH1  | 40:DF:119:ARG:HG2  | 2.32                     | 0.44              |
| 35:DA:2531:A:H4'   | 42:DH:157:TYR:CD2  | 2.53                     | 0.44              |
| 47:DO:119:PRO:O    | 47:DO:120:GLU:HB2  | 2.17                     | 0.44              |
| 47:DO:61:VAL:O     | 47:DO:84:ALA:HA    | 2.17                     | 0.44              |
| 48:DP:11:GLY:O     | 48:DP:12:ALA:O     | 2.36                     | 0.44              |
| 48:DP:83:VAL:CG1   | 48:DP:114:ILE:HA   | 2.47                     | 0.44              |
| 49:DQ:24:GLY:CA    | 49:DQ:67:ARG:HH12  | 2.30                     | 0.44              |
| 51:DS:89:ARG:CG    | 51:DS:92:TYR:CB    | 2.95                     | 0.44              |
| 52:DT:1:MET:H1     | 52:DT:7:ILE:HD11   | 1.81                     | 0.44              |
| 53:DU:15:LYS:HA    | 53:DU:18:LEU:HD12  | 1.99                     | 0.44              |
| 53:DU:102:GLU:HG3  | 54:DV:2:PHE:CE1    | 2.53                     | 0.44              |
| 54:DV:31:ALA:C     | 54:DV:61:VAL:HG12  | 2.37                     | 0.44              |
| 54:DV:89:GLN:OE1   | 54:DV:89:GLN:HA    | 2.18                     | 0.44              |
| 35:DA:300:A:P      | 57:DY:97:ARG:HE    | 2.40                     | 0.44              |
| 58:DZ:120:ILE:O    | 58:DZ:120:ILE:HG22 | 2.17                     | 0.44              |
| 58:DZ:99:TYR:HE2   | 58:DZ:125:LEU:HB2  | 1.82                     | 0.44              |
| 58:DZ:48:PHE:CD1   | 58:DZ:52:SER:HA    | 2.53                     | 0.44              |
| 58:DZ:29:TYR:O     | 58:DZ:90:VAL:HG23  | 2.18                     | 0.44              |
| 1:AA:103:C:H3'     | 1:AA:104:G:C8      | 2.43                     | 0.44              |
| 1:AA:1095:U:OP1    | 1:AA:1108:G:N2     | 2.50                     | 0.44              |
| 1:AA:1237:C:H5''   | 1:AA:1238:A:C8     | 2.53                     | 0.44              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:AA:559:A:OP2      | 5:AE:126:ARG:NH2   | 2.49                     | 0.44              |
| 1:AA:785:G:C2'      | 1:AA:786:G:H5'     | 2.48                     | 0.44              |
| 1:AA:80:G:N1        | 1:AA:90:U:H5'      | 2.32                     | 0.44              |
| 7:AG:108:ALA:O      | 7:AG:111:ARG:HB2   | 2.18                     | 0.44              |
| 7:AG:50:ILE:O       | 7:AG:54:THR:HG23   | 2.18                     | 0.44              |
| 9:AI:55:ALA:HA      | 9:AI:58:HIS:HD2    | 1.82                     | 0.44              |
| 10:AJ:63:PHE:N      | 10:AJ:63:PHE:CD2   | 2.82                     | 0.44              |
| 1:AA:1227:A:C2      | 13:AM:117:VAL:HG11 | 2.53                     | 0.44              |
| 13:AM:23:TYR:HE1    | 13:AM:70:LEU:HD22  | 1.83                     | 0.44              |
| 13:AM:49:THR:C      | 13:AM:51:ALA:N     | 2.70                     | 0.44              |
| 1:AA:1047:G:H5''    | 14:AN:4:LYS:HD3    | 2.00                     | 0.44              |
| 24:AY:204:GLU:O     | 24:AY:205:TYR:C    | 2.56                     | 0.44              |
| 24:AY:230:LYS:NZ    | 24:AY:237:PRO:HA   | 2.33                     | 0.44              |
| 24:AY:388:THR:HG21  | 24:AY:399:LEU:HD13 | 2.00                     | 0.44              |
| 24:AY:422:GLU:C     | 24:AY:424:LEU:N    | 2.68                     | 0.44              |
| 24:AY:25:LYS:HZ1    | 24:AY:86:GLY:HA2   | 1.83                     | 0.44              |
| 25:B0:3:HIS:NE2     | 35:BA:2602:A:H2    | 2.16                     | 0.44              |
| 26:B1:58:ILE:HD11   | 26:B1:91:LYS:HA    | 1.98                     | 0.44              |
| 26:B1:82:LEU:C      | 26:B1:83:GLU:CG    | 2.86                     | 0.44              |
| 33:B8:56:GLU:C      | 33:B8:58:ILE:N     | 2.70                     | 0.44              |
| 33:B8:59:LYS:HE3    | 33:B8:59:LYS:HB2   | 1.72                     | 0.44              |
| 34:B9:1:MET:SD      | 35:BA:2478:A:OP2   | 2.76                     | 0.44              |
| 34:B9:29:ASN:N      | 34:B9:29:ASN:HD22  | 2.15                     | 0.44              |
| 35:BA:143:G:H2'     | 35:BA:143(A):C:C6  | 2.53                     | 0.44              |
| 35:BA:1509(B):A:H2' | 35:BA:1510:G:C8    | 2.53                     | 0.44              |
| 35:BA:1582:C:O2'    | 35:BA:1583:A:H5'   | 2.17                     | 0.44              |
| 35:BA:1747(A):G:C2' | 35:BA:1748:G:C5'   | 2.75                     | 0.44              |
| 35:BA:1799:G:N2     | 35:BA:1818:U:H2'   | 2.33                     | 0.44              |
| 24:AY:580:MET:SD    | 35:BA:1913:A:C6    | 3.11                     | 0.44              |
| 35:BA:1963:U:C2'    | 35:BA:1963:U:O2    | 2.59                     | 0.44              |
| 35:BA:2140:C:H1'    | 35:BA:2152:G:N2    | 2.33                     | 0.44              |
| 35:BA:2150:U:H2'    | 35:BA:2151:G:H8    | 1.80                     | 0.44              |
| 31:B6:54:ILE:HD11   | 35:BA:2420:C:H5'   | 1.99                     | 0.44              |
| 35:BA:2696:U:H2'    | 35:BA:2697:G:C8    | 2.53                     | 0.44              |
| 35:BA:2754:U:C2'    | 35:BA:2755:C:H5'   | 2.48                     | 0.44              |
| 35:BA:2884:U:H2'    | 35:BA:2885:C:H5'   | 2.00                     | 0.44              |
| 35:BA:265:A:N6      | 35:BA:428:A:H1'    | 2.33                     | 0.44              |
| 35:BA:445:C:O2      | 35:BA:449:A:H2     | 2.00                     | 0.44              |
| 35:BA:483:A:C2      | 35:BA:484:C:H1'    | 2.53                     | 0.44              |
| 36:BB:89:G:N1       | 36:BB:90:A:C2      | 2.86                     | 0.44              |
| 38:BD:139:GLY:H     | 38:BD:165:ILE:HB   | 1.82                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 41:BG:46:ALA:HA    | 41:BG:51:ARG:HB3  | 1.99                     | 0.44              |
| 41:BG:58:GLN:C     | 41:BG:60:LEU:H    | 2.20                     | 0.44              |
| 42:BH:106:THR:HG22 | 42:BH:112:PRO:HB3 | 2.00                     | 0.44              |
| 42:BH:136:ILE:HG22 | 42:BH:136:ILE:O   | 2.18                     | 0.44              |
| 35:BA:2747:G:O2'   | 42:BH:67:LEU:HD12 | 2.17                     | 0.44              |
| 42:BH:35:VAL:CG2   | 42:BH:75:ALA:HB2  | 2.48                     | 0.44              |
| 42:BH:83:TYR:HB3   | 42:BH:134:SER:CA  | 2.39                     | 0.44              |
| 44:BK:106:GLU:HG3  | 44:BK:107:ILE:N   | 2.32                     | 0.44              |
| 44:BK:88:ALA:O     | 44:BK:90:LYS:N    | 2.42                     | 0.44              |
| 47:BO:37:ASP:O     | 47:BO:62:VAL:HG23 | 2.18                     | 0.44              |
| 35:BA:245:G:H5'    | 48:BP:73:GLY:HA2  | 2.00                     | 0.44              |
| 49:BQ:35:VAL:HG23  | 49:BQ:101:ARG:C   | 2.37                     | 0.44              |
| 54:BV:19:LYS:HZ1   | 54:BV:20:LEU:H    | 1.66                     | 0.44              |
| 54:BV:40:LEU:N     | 54:BV:40:LEU:HD22 | 2.32                     | 0.44              |
| 54:BV:47:VAL:O     | 54:BV:47:VAL:HG23 | 2.18                     | 0.44              |
| 57:BY:46:LYS:H     | 57:BY:62:GLU:CB   | 2.20                     | 0.44              |
| 58:BZ:119:GLU:C    | 58:BZ:121:HIS:N   | 2.68                     | 0.44              |
| 58:BZ:185:GLU:O    | 58:BZ:187:ALA:N   | 2.50                     | 0.44              |
| 1:CA:106:C:C2'     | 1:CA:107:G:H5'    | 2.48                     | 0.44              |
| 1:CA:1122:U:O2'    | 1:CA:1123:A:H5'   | 2.17                     | 0.44              |
| 1:CA:1351:U:H5'    | 7:CG:33:ASP:OD1   | 2.18                     | 0.44              |
| 1:CA:342:C:C5      | 1:CA:343:U:C5     | 3.06                     | 0.44              |
| 1:CA:472:A:H2'     | 1:CA:473:G:O4'    | 2.17                     | 0.44              |
| 1:CA:450:G:H1      | 1:CA:483:C:H42    | 1.65                     | 0.44              |
| 2:CB:209:ARG:HH11  | 2:CB:239:VAL:HG11 | 1.81                     | 0.44              |
| 3:CC:14:ILE:O      | 3:CC:15:THR:CB    | 2.66                     | 0.44              |
| 5:CE:26:PHE:N      | 5:CE:26:PHE:CD1   | 2.85                     | 0.44              |
| 7:CG:120:ILE:O     | 7:CG:124:LEU:HD12 | 2.18                     | 0.44              |
| 7:CG:65:ALA:HA     | 7:CG:128:ALA:CA   | 2.47                     | 0.44              |
| 7:CG:129:GLU:OE2   | 7:CG:131:LYS:HE2  | 2.17                     | 0.44              |
| 9:CI:42:ARG:O      | 9:CI:44:VAL:N     | 2.50                     | 0.44              |
| 9:CI:4:TYR:CE1     | 9:CI:88:TYR:CD2   | 3.05                     | 0.44              |
| 9:CI:114:TYR:HD1   | 10:CJ:60:ARG:HG3  | 1.83                     | 0.44              |
| 10:CJ:37:PRO:CA    | 10:CJ:72:VAL:HG22 | 2.39                     | 0.44              |
| 10:CJ:81:THR:C     | 10:CJ:83:GLU:N    | 2.69                     | 0.44              |
| 11:CK:120:ARG:NH1  | 11:CK:126:ARG:NE  | 2.66                     | 0.44              |
| 17:CQ:99:SER:O     | 17:CQ:100:LYS:HG3 | 2.18                     | 0.44              |
| 19:CS:35:SER:C     | 19:CS:37:ARG:N    | 2.71                     | 0.44              |
| 24:CY:117:GLN:OE1  | 24:CY:120:THR:OG1 | 2.36                     | 0.44              |
| 24:CY:125:ALA:C    | 24:CY:127:LYS:H   | 2.22                     | 0.44              |
| 24:CY:484:ARG:HD3  | 24:CY:484:ARG:HA  | 1.79                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:CY:673:PHE:CE2 | 24:CY:674:ASP:O    | 2.71                     | 0.44              |
| 24:CY:602:LEU:HB3 | 24:CY:676:TYR:HB3  | 1.99                     | 0.44              |
| 25:D0:3:HIS:NE2   | 35:DA:2602:A:H2    | 2.16                     | 0.44              |
| 31:D6:24:GLU:HG3  | 31:D6:37:ARG:HH21  | 1.83                     | 0.44              |
| 35:DA:1227:G:O2'  | 35:DA:1228:G:H5'   | 2.18                     | 0.44              |
| 35:DA:1213:A:N3   | 35:DA:1238:G:H1'   | 2.32                     | 0.44              |
| 35:DA:1408:C:H42  | 35:DA:1594:G:H1    | 1.66                     | 0.44              |
| 35:DA:1495:A:N3   | 35:DA:1496:A:C2    | 2.85                     | 0.44              |
| 35:DA:1657:C:H2'  | 35:DA:1658:C:C6    | 2.53                     | 0.44              |
| 35:DA:1680:U:O2'  | 35:DA:1681:G:H5'   | 2.18                     | 0.44              |
| 35:DA:2088:G:C6   | 35:DA:2089:U:C4    | 3.06                     | 0.44              |
| 35:DA:2148:G:O2'  | 35:DA:2149:G:H5'   | 2.18                     | 0.44              |
| 35:DA:2307:G:H3'  | 35:DA:2308:G:C5'   | 2.47                     | 0.44              |
| 35:DA:2328:A:O5'  | 35:DA:2328:A:H8    | 2.01                     | 0.44              |
| 35:DA:2334:G:N3   | 51:DS:18:ILE:HD13  | 2.33                     | 0.44              |
| 35:DA:2523:G:C3'  | 35:DA:2524:G:H5''  | 2.46                     | 0.44              |
| 35:DA:2688:U:O2   | 35:DA:2688:U:H3'   | 2.17                     | 0.44              |
| 35:DA:272(I):U:H5 | 35:DA:363(A):A:C2  | 2.35                     | 0.44              |
| 35:DA:338:G:H2'   | 35:DA:339:U:H6     | 1.82                     | 0.44              |
| 35:DA:602:G:N1    | 35:DA:654(U):A:N7  | 2.65                     | 0.44              |
| 35:DA:619:G:H3'   | 35:DA:620:G:N2     | 2.32                     | 0.44              |
| 35:DA:775:G:C4    | 35:DA:794:G:C8     | 3.05                     | 0.44              |
| 35:DA:84:A:H5''   | 57:DY:9:LYS:HZ3    | 1.79                     | 0.44              |
| 35:DA:892:G:O2'   | 35:DA:893:C:H5'    | 2.17                     | 0.44              |
| 35:DA:972:G:OP2   | 35:DA:974:G:H5''   | 2.18                     | 0.44              |
| 36:DB:58:A:H2'    | 36:DB:59:A:O4'     | 2.18                     | 0.44              |
| 36:DB:4:C:H2'     | 36:DB:5:C:C6       | 2.53                     | 0.44              |
| 35:DA:919:G:H5'   | 36:DB:81:G:H1'     | 2.00                     | 0.44              |
| 37:DC:138:LEU:O   | 37:DC:138:LEU:HD13 | 2.18                     | 0.44              |
| 38:DD:117:VAL:CG2 | 38:DD:118:VAL:N    | 2.81                     | 0.44              |
| 39:DE:119:ARG:HD2 | 39:DE:120:TRP:CE2  | 2.53                     | 0.44              |
| 39:DE:177:PRO:O   | 39:DE:178:GLU:C    | 2.56                     | 0.44              |
| 39:DE:36:ARG:HH21 | 39:DE:88:GLY:HA2   | 1.79                     | 0.44              |
| 40:DF:109:GLY:HA2 | 40:DF:112:MET:HB2  | 1.99                     | 0.44              |
| 40:DF:20:LEU:HD23 | 40:DF:21:ALA:H     | 1.83                     | 0.44              |
| 41:DG:6:ALA:O     | 41:DG:10:LYS:HB2   | 2.17                     | 0.44              |
| 41:DG:133:LEU:C   | 41:DG:133:LEU:HD12 | 2.38                     | 0.44              |
| 46:DN:15:LEU:O    | 46:DN:136:GLU:HA   | 2.18                     | 0.44              |
| 48:DP:89:ALA:O    | 48:DP:121:LYS:HD2  | 2.17                     | 0.44              |
| 49:DQ:54:MET:CG   | 49:DQ:64:ILE:HD13  | 2.40                     | 0.44              |
| 50:DR:24:GLN:NE2  | 50:DR:36:THR:HG21  | 2.32                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 52:DT:26:ASP:OD2   | 52:DT:26:ASP:O    | 2.36                     | 0.44              |
| 52:DT:27:THR:C     | 52:DT:28:VAL:HG23 | 2.37                     | 0.44              |
| 52:DT:29:ARG:CD    | 52:DT:86:ILE:HG22 | 2.48                     | 0.44              |
| 54:DV:19:LYS:HZ3   | 54:DV:20:LEU:H    | 1.64                     | 0.44              |
| 57:DY:77:PRO:O     | 57:DY:99:CYS:SG   | 2.71                     | 0.44              |
| 58:DZ:11:GLU:H     | 58:DZ:11:GLU:CD   | 2.21                     | 0.44              |
| 58:DZ:180:VAL:HG12 | 58:DZ:181:GLU:N   | 2.33                     | 0.44              |
| 58:DZ:179:ASP:OD1  | 58:DZ:181:GLU:N   | 2.51                     | 0.44              |
| 1:AA:109:A:C6      | 1:AA:326:G:C6     | 3.05                     | 0.44              |
| 1:AA:1165:C:C4     | 1:AA:1166:G:N7    | 2.85                     | 0.44              |
| 1:AA:1388:C:H2'    | 1:AA:1389:C:C6    | 2.52                     | 0.44              |
| 1:AA:17:U:H1'      | 1:AA:1080:A:N3    | 2.32                     | 0.44              |
| 1:AA:316:G:C6      | 1:AA:338:A:C6     | 3.05                     | 0.44              |
| 1:AA:403:C:H2'     | 1:AA:404:U:H6     | 1.83                     | 0.44              |
| 1:AA:644:G:C5      | 1:AA:645:C:C5     | 3.05                     | 0.44              |
| 1:AA:663:A:C2'     | 1:AA:664:G:H5'    | 2.48                     | 0.44              |
| 1:AA:979:C:C2'     | 1:AA:980:C:H5''   | 2.44                     | 0.44              |
| 1:AA:98:G:C2'      | 1:AA:99:U:H5'     | 2.48                     | 0.44              |
| 2:AB:21:ARG:O      | 2:AB:22:LYS:HB2   | 2.18                     | 0.44              |
| 2:AB:51:LEU:O      | 2:AB:55:PHE:HD2   | 2.00                     | 0.44              |
| 3:AC:43:LEU:C      | 3:AC:45:LYS:H     | 2.21                     | 0.44              |
| 4:AD:144:ASP:O     | 4:AD:184:LYS:HA   | 2.16                     | 0.44              |
| 5:AE:64:ARG:NH1    | 5:AE:64:ARG:CG    | 2.73                     | 0.44              |
| 9:AI:43:ALA:O      | 9:AI:45:ALA:N     | 2.51                     | 0.44              |
| 1:AA:1371:G:O3'    | 9:AI:69:GLY:HA3   | 2.17                     | 0.44              |
| 10:AJ:5:ARG:HG3    | 10:AJ:71:LEU:HD11 | 1.99                     | 0.44              |
| 11:AK:60:ALA:O     | 11:AK:61:ALA:C    | 2.57                     | 0.44              |
| 1:AA:953:G:N7      | 13:AM:104:ARG:NH2 | 2.65                     | 0.44              |
| 18:AR:69:THR:O     | 18:AR:72:ARG:HB2  | 2.18                     | 0.44              |
| 24:AY:20:HIS:CD2   | 24:AY:117:GLN:HB3 | 2.53                     | 0.44              |
| 24:AY:686:LYS:HD3  | 24:AY:686:LYS:C   | 2.39                     | 0.44              |
| 25:B0:49:LYS:HG3   | 25:B0:80:HIS:ND1  | 2.32                     | 0.44              |
| 28:B3:46:ASN:O     | 28:B3:47:VAL:C    | 2.54                     | 0.44              |
| 35:BA:1488:G:H5'   | 35:BA:1489:U:OP2  | 2.17                     | 0.44              |
| 35:BA:1710:C:H2'   | 35:BA:1711:C:C6   | 2.53                     | 0.44              |
| 35:BA:200:U:C2'    | 35:BA:201:C:H5'   | 2.48                     | 0.44              |
| 35:BA:2131:G:C8    | 35:BA:2133:G:C2   | 3.06                     | 0.44              |
| 35:BA:2309:A:H2'   | 35:BA:2310:A:H5'' | 1.99                     | 0.44              |
| 35:BA:2514:U:H2'   | 35:BA:2515:C:C6   | 2.38                     | 0.44              |
| 35:BA:2767:C:H2'   | 35:BA:2768:C:C6   | 2.52                     | 0.44              |
| 35:BA:285:C:H2'    | 35:BA:286:C:C5'   | 2.48                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:2880:C:N4    | 35:BA:2881:C:H41   | 2.15                     | 0.44              |
| 35:BA:465:G:H2'    | 35:BA:466:A:C8     | 2.53                     | 0.44              |
| 35:BA:665:C:O2'    | 35:BA:666:G:H5'    | 2.16                     | 0.44              |
| 35:BA:949:C:H2'    | 35:BA:950:G:H8     | 1.82                     | 0.44              |
| 38:BD:145:VAL:HG22 | 38:BD:191:ALA:CB   | 2.39                     | 0.44              |
| 38:BD:176:ARG:CG   | 38:BD:176:ARG:NH1  | 2.77                     | 0.44              |
| 38:BD:39:LYS:HZ1   | 38:BD:87:ASN:HB3   | 1.82                     | 0.44              |
| 39:BE:50:GLY:HA3   | 39:BE:74:PRO:HG3   | 2.00                     | 0.44              |
| 41:BG:107:LEU:HD23 | 41:BG:111:LEU:HD12 | 1.99                     | 0.44              |
| 41:BG:135:LEU:HD12 | 41:BG:135:LEU:N    | 2.31                     | 0.44              |
| 42:BH:130:ARG:NH1  | 42:BH:130:ARG:HB3  | 2.33                     | 0.44              |
| 42:BH:38:SER:C     | 42:BH:40:GLU:H     | 2.21                     | 0.44              |
| 42:BH:56:SER:HG    | 42:BH:61:HIS:CE1   | 2.31                     | 0.44              |
| 42:BH:83:TYR:HA    | 42:BH:135:GLY:O    | 2.18                     | 0.44              |
| 46:BN:62:VAL:HG22  | 46:BN:66:LYS:CG    | 2.41                     | 0.44              |
| 48:BP:98:GLU:HA    | 48:BP:101:VAL:HG22 | 1.98                     | 0.44              |
| 49:BQ:27:VAL:O     | 49:BQ:28:ALA:CB    | 2.66                     | 0.44              |
| 49:BQ:65:PHE:N     | 49:BQ:65:PHE:CD2   | 2.86                     | 0.44              |
| 49:BQ:78:PRO:HB2   | 49:BQ:81:VAL:HG11  | 2.00                     | 0.44              |
| 50:BR:97:VAL:HG13  | 50:BR:114:VAL:CG2  | 2.48                     | 0.44              |
| 52:BT:13:ARG:HA    | 52:BT:13:ARG:NE    | 2.31                     | 0.44              |
| 53:BU:82:GLY:C     | 53:BU:84:LYS:N     | 2.71                     | 0.44              |
| 54:BV:35:LEU:HB3   | 54:BV:37:VAL:HG23  | 1.99                     | 0.44              |
| 54:BV:46:VAL:HG22  | 54:BV:47:VAL:N     | 2.28                     | 0.44              |
| 54:BV:39:LEU:HD13  | 54:BV:51:VAL:HA    | 1.99                     | 0.44              |
| 35:BA:64:A:C5      | 56:BX:66:LEU:HD13  | 2.53                     | 0.44              |
| 1:CA:1037:C:H2'    | 1:CA:1038:C:N1     | 2.32                     | 0.44              |
| 1:CA:1053:G:O6     | 1:CA:1199:U:H2'    | 2.17                     | 0.44              |
| 1:CA:1132:C:N4     | 1:CA:1133:G:C6     | 2.86                     | 0.44              |
| 1:CA:1316:G:O3'    | 14:CN:18:VAL:CG1   | 2.66                     | 0.44              |
| 1:CA:791:G:N2      | 1:CA:1497:G:O3'    | 2.49                     | 0.44              |
| 1:CA:408:A:OP1     | 4:CD:113:SER:OG    | 2.25                     | 0.44              |
| 1:CA:432:A:N7      | 1:CA:433:C:C4      | 2.86                     | 0.44              |
| 1:CA:625:G:H4'     | 16:CP:16:HIS:HD2   | 1.81                     | 0.44              |
| 1:CA:637:G:O2'     | 1:CA:638:G:H5'     | 2.17                     | 0.44              |
| 1:CA:769:G:O2'     | 1:CA:770:C:H5'     | 2.18                     | 0.44              |
| 2:CB:114:ARG:O     | 2:CB:117:GLU:HB2   | 2.17                     | 0.44              |
| 2:CB:223:ILE:C     | 2:CB:225:ALA:N     | 2.70                     | 0.44              |
| 2:CB:229:VAL:HG12  | 2:CB:230:VAL:N     | 2.33                     | 0.44              |
| 3:CC:110:ASN:HD21  | 3:CC:140:ARG:HB3   | 1.83                     | 0.44              |
| 3:CC:87:LEU:C      | 3:CC:89:GLU:N      | 2.70                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:CD:92:VAL:O      | 4:CD:95:GLY:N     | 2.51                     | 0.44              |
| 5:CE:155:GLU:N     | 8:CH:46:LYS:HG2   | 2.33                     | 0.44              |
| 8:CH:114:THR:C     | 8:CH:116:LYS:H    | 2.21                     | 0.44              |
| 8:CH:44:PHE:HE2    | 8:CH:109:ILE:HG21 | 1.82                     | 0.44              |
| 11:CK:58:PRO:HA    | 11:CK:90:GLY:CA   | 2.44                     | 0.44              |
| 12:CL:50:SER:O     | 12:CL:51:ALA:HB2  | 2.18                     | 0.44              |
| 14:CN:12:ARG:HB2   | 14:CN:12:ARG:NH1  | 2.33                     | 0.44              |
| 21:CU:8:THR:O      | 21:CU:9:ARG:C     | 2.55                     | 0.44              |
| 22:CW:14:A:H3'     | 22:CW:15:G:C5'    | 2.47                     | 0.44              |
| 24:CY:136:ALA:CB   | 24:CY:260:LEU:HB3 | 2.28                     | 0.44              |
| 24:CY:519:ARG:NH1  | 24:CY:678:GLU:HB2 | 2.33                     | 0.44              |
| 24:CY:461:ILE:HD11 | 61:CY:702:FUA:H21 | 2.00                     | 0.44              |
| 27:D2:57:ILE:H     | 27:D2:57:ILE:HG12 | 1.47                     | 0.44              |
| 29:D4:7:PRO:O      | 29:D4:8:LYS:HB3   | 2.18                     | 0.44              |
| 32:D7:48:LYS:NZ    | 35:DA:125:G:N2    | 2.66                     | 0.44              |
| 35:DA:55:G:H1      | 35:DA:115:C:H42   | 1.65                     | 0.44              |
| 35:DA:1598:C:H2'   | 35:DA:1599:C:C6   | 2.53                     | 0.44              |
| 35:DA:1719:G:O2'   | 35:DA:1720:U:H5'  | 2.17                     | 0.44              |
| 35:DA:2147:G:H2'   | 35:DA:2148:G:C5'  | 2.48                     | 0.44              |
| 35:DA:2193:G:H8    | 35:DA:2193:G:H5'  | 1.82                     | 0.44              |
| 35:DA:21:A:O2'     | 35:DA:22:C:H5'    | 2.18                     | 0.44              |
| 35:DA:2341:G:H2'   | 35:DA:2342:C:C6   | 2.52                     | 0.44              |
| 35:DA:2547:U:H2'   | 35:DA:2548:G:H8   | 1.82                     | 0.44              |
| 35:DA:2550:G:C6    | 35:DA:2551:C:N4   | 2.86                     | 0.44              |
| 35:DA:2628:C:O2'   | 35:DA:2781:A:H2'  | 2.17                     | 0.44              |
| 35:DA:2876:G:OP1   | 52:DT:2:ASN:O     | 2.36                     | 0.44              |
| 35:DA:526:A:N6     | 35:DA:2626:C:H4'  | 2.32                     | 0.44              |
| 35:DA:795:C:H2'    | 35:DA:796:C:C6    | 2.52                     | 0.44              |
| 37:DC:101:ILE:H    | 37:DC:101:ILE:CD1 | 2.28                     | 0.44              |
| 37:DC:23:ILE:CB    | 37:DC:229:SER:OXT | 2.62                     | 0.44              |
| 37:DC:76:LEU:HB3   | 37:DC:114:VAL:HA  | 2.00                     | 0.44              |
| 37:DC:88:GLU:N     | 37:DC:95:VAL:HG21 | 2.32                     | 0.44              |
| 39:DE:201:THR:C    | 39:DE:202:LYS:HD2 | 2.37                     | 0.44              |
| 39:DE:2:LYS:CD     | 39:DE:95:ILE:HG22 | 2.47                     | 0.44              |
| 39:DE:68:ALA:C     | 39:DE:70:ALA:H    | 2.21                     | 0.44              |
| 40:DF:20:LEU:HD13  | 40:DF:203:GLN:OE1 | 2.18                     | 0.44              |
| 41:DG:86:MET:HG2   | 41:DG:86:MET:O    | 2.18                     | 0.44              |
| 35:DA:2653:U:O2'   | 42:DH:110:SER:CB  | 2.66                     | 0.44              |
| 42:DH:76:VAL:C     | 42:DH:78:GLY:H    | 2.21                     | 0.44              |
| 44:DK:75:SER:C     | 44:DK:78:ILE:HG22 | 2.38                     | 0.44              |
| 48:DP:144:GLU:N    | 48:DP:145:PRO:HD3 | 2.33                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:DP:7:ARG:CB     | 48:DP:8:PRO:CD     | 2.95                     | 0.44              |
| 51:DS:48:LEU:N     | 51:DS:48:LEU:HD12  | 2.33                     | 0.44              |
| 52:DT:57:PHE:CG    | 52:DT:58:ASN:N     | 2.85                     | 0.44              |
| 52:DT:92:GLY:C     | 52:DT:94:ALA:N     | 2.70                     | 0.44              |
| 57:DY:9:LYS:O      | 57:DY:28:LYS:HE2   | 2.17                     | 0.44              |
| 58:DZ:157:LEU:HD11 | 58:DZ:163:LEU:HD22 | 1.99                     | 0.44              |
| 58:DZ:171:ILE:CG1  | 58:DZ:172:ALA:N    | 2.81                     | 0.44              |
| 1:AA:829:G:O2'     | 1:AA:830:G:H5'     | 2.18                     | 0.43              |
| 2:AB:142:LEU:HD23  | 2:AB:142:LEU:C     | 2.38                     | 0.43              |
| 2:AB:214:ILE:O     | 2:AB:218:ALA:HB2   | 2.17                     | 0.43              |
| 3:AC:130:VAL:O     | 3:AC:134:ILE:HG13  | 2.18                     | 0.43              |
| 3:AC:182:ILE:HG12  | 3:AC:203:PHE:HD1   | 1.82                     | 0.43              |
| 4:AD:134:ASP:N     | 4:AD:134:ASP:OD2   | 2.49                     | 0.43              |
| 5:AE:142:LEU:O     | 5:AE:143:ARG:CD    | 2.66                     | 0.43              |
| 7:AG:84:ASN:ND2    | 7:AG:84:ASN:N      | 2.65                     | 0.43              |
| 8:AH:17:THR:CG2    | 8:AH:63:LEU:HD12   | 2.48                     | 0.43              |
| 9:AI:111:ARG:HG2   | 9:AI:112:LYS:N     | 2.33                     | 0.43              |
| 9:AI:60:ASP:O      | 9:AI:61:ALA:O      | 2.36                     | 0.43              |
| 10:AJ:90:LEU:H     | 10:AJ:91:PRO:HD3   | 1.82                     | 0.43              |
| 11:AK:58:PRO:HA    | 11:AK:90:GLY:CA    | 2.45                     | 0.43              |
| 12:AL:91:LYS:HB2   | 12:AL:91:LYS:HE2   | 1.69                     | 0.43              |
| 13:AM:91:ARG:HD3   | 13:AM:97:PRO:O     | 2.18                     | 0.43              |
| 14:AN:24:CYS:SG    | 14:AN:25:VAL:N     | 2.91                     | 0.43              |
| 14:AN:48:ALA:HB2   | 14:AN:53:LEU:HD12  | 1.99                     | 0.43              |
| 1:AA:1115:C:H1'    | 14:AN:61:TRP:O     | 2.18                     | 0.43              |
| 15:AO:9:GLN:O      | 15:AO:11:VAL:N     | 2.51                     | 0.43              |
| 24:AY:219:VAL:C    | 24:AY:221:ALA:N    | 2.72                     | 0.43              |
| 24:AY:635:GLU:CD   | 24:AY:635:GLU:N    | 2.71                     | 0.43              |
| 27:B2:9:GLN:O      | 27:B2:13:ALA:N     | 2.45                     | 0.43              |
| 30:B5:55:ARG:HH22  | 50:BR:33:ARG:CG    | 2.29                     | 0.43              |
| 35:BA:152:G:H1     | 35:BA:174:C:H42    | 1.66                     | 0.43              |
| 35:BA:1541:G:H5''  | 35:BA:1542:A:OP1   | 2.18                     | 0.43              |
| 35:BA:153:C:H2'    | 35:BA:154:G:C8     | 2.53                     | 0.43              |
| 35:BA:15:G:H2'     | 35:BA:16:G:H8      | 1.83                     | 0.43              |
| 35:BA:1801:G:H3'   | 35:BA:1802:A:H5'   | 2.00                     | 0.43              |
| 35:BA:1805:U:H2'   | 35:BA:1806:C:C6    | 2.52                     | 0.43              |
| 35:BA:1810:A:H2'   | 35:BA:1811:G:O4'   | 2.17                     | 0.43              |
| 35:BA:1843:C:H2'   | 35:BA:1844:C:C6    | 2.53                     | 0.43              |
| 35:BA:1993:U:C5'   | 39:BE:128:SER:HB3  | 2.48                     | 0.43              |
| 35:BA:2154:G:H2'   | 35:BA:2155:G:C8    | 2.53                     | 0.43              |
| 35:BA:2131:G:H8    | 35:BA:2158:A:H62   | 1.64                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:2219:G:O5'   | 35:BA:2219:G:H8    | 2.01                     | 0.43              |
| 35:BA:2282:G:O2'   | 35:BA:2283:C:OP2   | 2.29                     | 0.43              |
| 35:BA:2419:U:O2'   | 35:BA:2420:C:H5'   | 2.17                     | 0.43              |
| 35:BA:268:C:O2     | 35:BA:268:C:H2'    | 2.17                     | 0.43              |
| 35:BA:269:U:H2'    | 35:BA:270:A:H8     | 1.82                     | 0.43              |
| 35:BA:37:C:H2'     | 35:BA:37:C:O2      | 2.17                     | 0.43              |
| 35:BA:458:G:N2     | 35:BA:469:G:H2'    | 2.32                     | 0.43              |
| 35:BA:706:A:H2'    | 35:BA:707:G:O4'    | 2.18                     | 0.43              |
| 35:BA:848:G:H5''   | 35:BA:928:G:N2     | 2.33                     | 0.43              |
| 37:BC:138:LEU:HD13 | 37:BC:138:LEU:O    | 2.17                     | 0.43              |
| 37:BC:223:VAL:HG12 | 37:BC:225:ILE:HG23 | 2.00                     | 0.43              |
| 38:BD:34:VAL:O     | 38:BD:36:PRO:CD    | 2.67                     | 0.43              |
| 39:BE:96:PHE:HA    | 39:BE:100:GLU:OE1  | 2.19                     | 0.43              |
| 35:BA:2572:A:C8    | 39:BE:144:ARG:CB   | 3.01                     | 0.43              |
| 40:BF:102:PRO:HB2  | 40:BF:105:VAL:HG23 | 1.99                     | 0.43              |
| 48:BP:71:VAL:CG1   | 48:BP:72:PRO:HD3   | 2.47                     | 0.43              |
| 52:BT:30:VAL:HG21  | 52:BT:83:ILE:CG1   | 2.48                     | 0.43              |
| 52:BT:32:TYR:HB3   | 52:BT:81:PRO:HB2   | 1.98                     | 0.43              |
| 58:BZ:72:ARG:HD3   | 58:BZ:72:ARG:HA    | 1.78                     | 0.43              |
| 1:CA:1165:C:C4     | 1:CA:1166:G:N7     | 2.86                     | 0.43              |
| 1:CA:1202:G:O2'    | 1:CA:1203:C:H5'    | 2.17                     | 0.43              |
| 1:CA:720:C:C3'     | 1:CA:721:G:H5''    | 2.37                     | 0.43              |
| 1:CA:833:U:H2'     | 1:CA:834:C:H6      | 1.81                     | 0.43              |
| 1:CA:954:G:H2'     | 1:CA:955:U:H6      | 1.79                     | 0.43              |
| 1:CA:972:C:O2'     | 10:CJ:55:LYS:HB3   | 2.18                     | 0.43              |
| 3:CC:129:ALA:C     | 3:CC:131:ARG:N     | 2.70                     | 0.43              |
| 4:CD:173:TRP:CB    | 4:CD:187:ARG:NH1   | 2.81                     | 0.43              |
| 7:CG:80:VAL:CG2    | 7:CG:81:GLY:N      | 2.80                     | 0.43              |
| 10:CJ:30:SER:HA    | 10:CJ:80:LYS:CE    | 2.48                     | 0.43              |
| 10:CJ:61:GLU:HG3   | 14:CN:58:LYS:HE2   | 2.00                     | 0.43              |
| 10:CJ:98:ILE:CG2   | 10:CJ:98:ILE:O     | 2.66                     | 0.43              |
| 11:CK:66:LEU:HD23  | 11:CK:66:LEU:HA    | 1.81                     | 0.43              |
| 1:CA:539:A:OP2     | 12:CL:115:LYS:HE3  | 2.17                     | 0.43              |
| 12:CL:70:ILE:HG23  | 12:CL:100:ILE:HD12 | 1.99                     | 0.43              |
| 14:CN:42:ILE:HA    | 14:CN:42:ILE:HD13  | 1.66                     | 0.43              |
| 15:CO:74:ASP:C     | 15:CO:76:GLU:N     | 2.70                     | 0.43              |
| 17:CQ:43:LEU:HD23  | 17:CQ:43:LEU:HA    | 1.74                     | 0.43              |
| 19:CS:57:HIS:O     | 19:CS:59:PRO:HD3   | 2.17                     | 0.43              |
| 22:CV:35:A:C2'     | 22:CV:36:U:H5'     | 2.48                     | 0.43              |
| 24:CY:210:ARG:O    | 24:CY:213:HIS:N    | 2.51                     | 0.43              |
| 24:CY:613:PRO:HG2  | 24:CY:666:ARG:HH21 | 1.82                     | 0.43              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:D0:23:VAL:HA    | 25:D0:38:VAL:HG13  | 2.00                     | 0.43              |
| 25:D0:19:LYS:CD    | 25:D0:41:ARG:HH22  | 2.28                     | 0.43              |
| 30:D5:2:ALA:CA     | 35:DA:2015:A:C1'   | 2.86                     | 0.43              |
| 31:D6:28:ARG:HB2   | 31:D6:29:ASN:H     | 1.63                     | 0.43              |
| 31:D6:7:ILE:O      | 31:D6:7:ILE:HG22   | 2.18                     | 0.43              |
| 33:D8:32:LEU:O     | 33:D8:33:ASN:O     | 2.36                     | 0.43              |
| 35:DA:1185:C:C5'   | 35:DA:1186:G:P     | 3.06                     | 0.43              |
| 35:DA:1488:G:H5'   | 35:DA:1489:U:OP2   | 2.18                     | 0.43              |
| 35:DA:1801:G:H3'   | 35:DA:1802:A:H5'   | 1.98                     | 0.43              |
| 35:DA:2050:C:H1'   | 39:DE:156:MET:HE1  | 1.98                     | 0.43              |
| 35:DA:2337:G:H2'   | 35:DA:2338:G:C8    | 2.53                     | 0.43              |
| 35:DA:2439:A:C8    | 35:DA:2586:C:H4'   | 2.53                     | 0.43              |
| 35:DA:2443:C:C2'   | 35:DA:2443:C:O2    | 2.65                     | 0.43              |
| 35:DA:27:G:H1'     | 35:DA:513:A:N6     | 2.33                     | 0.43              |
| 35:DA:708:C:H42    | 35:DA:723:G:H1     | 1.66                     | 0.43              |
| 35:DA:856:C:H2'    | 35:DA:857:C:C6     | 2.53                     | 0.43              |
| 35:DA:947:G:N3     | 35:DA:984:A:H2     | 2.16                     | 0.43              |
| 35:DA:959:A:N1     | 35:DA:960:A:C2     | 2.86                     | 0.43              |
| 36:DB:86:G:H2'     | 36:DB:87:G:H8      | 1.79                     | 0.43              |
| 36:DB:96:U:H2'     | 36:DB:97:G:H8      | 1.84                     | 0.43              |
| 37:DC:140:ASN:H    | 37:DC:145:THR:HB   | 1.83                     | 0.43              |
| 38:DD:8:PRO:C      | 38:DD:10:THR:H     | 2.20                     | 0.43              |
| 39:DE:14:ILE:HD11  | 39:DE:173:VAL:HG11 | 1.99                     | 0.43              |
| 40:DF:89:VAL:CG1   | 40:DF:90:PHE:H     | 2.26                     | 0.43              |
| 41:DG:121:ASN:OD1  | 41:DG:123:ASN:N    | 2.49                     | 0.43              |
| 42:DH:66:GLY:CA    | 42:DH:69:ARG:HB3   | 2.42                     | 0.43              |
| 45:DL:26:UNK:C     | 45:DL:28:UNK:H     | 2.31                     | 0.43              |
| 46:DN:67:LEU:O     | 46:DN:68:GLU:CB    | 2.61                     | 0.43              |
| 47:DO:88:ASN:C     | 47:DO:90:GLN:H     | 2.22                     | 0.43              |
| 48:DP:81:GLN:HG2   | 48:DP:106:LEU:HA   | 2.00                     | 0.43              |
| 48:DP:71:VAL:CG1   | 48:DP:72:PRO:HD3   | 2.48                     | 0.43              |
| 51:DS:28:VAL:HG13  | 51:DS:36:TYR:O     | 2.18                     | 0.43              |
| 54:DV:39:LEU:HD12  | 54:DV:47:VAL:HG11  | 2.00                     | 0.43              |
| 55:DW:70:TYR:HB3   | 55:DW:110:LYS:NZ   | 2.33                     | 0.43              |
| 57:DY:103:GLY:O    | 57:DY:105:ALA:N    | 2.51                     | 0.43              |
| 57:DY:96:ILE:HG21  | 57:DY:99:CYS:HB3   | 2.00                     | 0.43              |
| 58:DZ:102:LEU:HD21 | 58:DZ:124:ILE:HD13 | 1.99                     | 0.43              |
| 58:DZ:151:HIS:HB2  | 58:DZ:168:GLU:O    | 2.18                     | 0.43              |
| 1:AA:1354:C:H2'    | 1:AA:1355:G:H8     | 1.82                     | 0.43              |
| 1:AA:149:A:H2'     | 1:AA:149:A:N3      | 2.33                     | 0.43              |
| 1:AA:961:U:O2'     | 1:AA:962:C:H5'     | 2.18                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:AB:223:ILE:C     | 2:AB:225:ALA:N     | 2.70                     | 0.43              |
| 3:AC:109:PRO:CD    | 3:AC:110:ASN:H     | 2.31                     | 0.43              |
| 3:AC:80:GLY:CA     | 3:AC:82:GLU:OE1    | 2.66                     | 0.43              |
| 4:AD:96:LEU:O      | 4:AD:97:LEU:C      | 2.56                     | 0.43              |
| 5:AE:76:ILE:HG22   | 5:AE:118:ILE:HD13  | 1.99                     | 0.43              |
| 9:AI:79:LEU:O      | 9:AI:82:ALA:N      | 2.52                     | 0.43              |
| 11:AK:116:HIS:O    | 11:AK:117:ASN:HB2  | 2.18                     | 0.43              |
| 16:AP:14:ASN:N     | 16:AP:15:PRO:CD    | 2.81                     | 0.43              |
| 18:AR:36:ASN:OD1   | 18:AR:39:VAL:HB    | 2.18                     | 0.43              |
| 19:AS:19:VAL:HG12  | 19:AS:20:LEU:N     | 2.33                     | 0.43              |
| 24:AY:152:THR:HA   | 24:AY:155:GLU:HB3  | 1.99                     | 0.43              |
| 24:AY:614:GLU:HA   | 24:AY:617:MET:CB   | 2.47                     | 0.43              |
| 24:AY:87:HIS:NE2   | 24:AY:120:THR:HG21 | 2.32                     | 0.43              |
| 25:B0:70:GLN:NE2   | 25:B0:80:HIS:NE2   | 2.66                     | 0.43              |
| 26:B1:89:GLU:O     | 26:B1:93:GLU:HG2   | 2.18                     | 0.43              |
| 29:B4:1:MET:HG2    | 41:BG:98:ARG:CD    | 2.48                     | 0.43              |
| 31:B6:29:ASN:CG    | 31:B6:30:THR:N     | 2.70                     | 0.43              |
| 33:B8:58:ILE:CG2   | 48:BP:49:ARG:HD3   | 2.48                     | 0.43              |
| 35:BA:1328:G:H2'   | 35:BA:1330:C:C5    | 2.54                     | 0.43              |
| 35:BA:1362:C:H2'   | 35:BA:1363:C:C6    | 2.53                     | 0.43              |
| 35:BA:1485:G:H5'   | 35:BA:1485:G:H8    | 1.82                     | 0.43              |
| 35:BA:1487:G:N3    | 35:BA:1487:G:H2'   | 2.34                     | 0.43              |
| 35:BA:1495:A:H2'   | 35:BA:1495:A:N3    | 2.33                     | 0.43              |
| 35:BA:2688:U:H1'   | 35:BA:2721:A:H61   | 1.82                     | 0.43              |
| 35:BA:272(H):C:H5' | 35:BA:272(H):C:C6  | 2.34                     | 0.43              |
| 35:BA:2836:U:C4    | 35:BA:2883:A:N6    | 2.86                     | 0.43              |
| 39:BE:26:ILE:HG13  | 39:BE:182:LEU:HB3  | 2.00                     | 0.43              |
| 40:BF:206:ILE:CG2  | 40:BF:207:GLY:N    | 2.81                     | 0.43              |
| 41:BG:107:LEU:HD23 | 41:BG:111:LEU:HD11 | 2.00                     | 0.43              |
| 41:BG:170:ARG:HE   | 41:BG:180:PHE:HD1  | 1.65                     | 0.43              |
| 48:BP:106:LEU:N    | 48:BP:106:LEU:HD12 | 2.33                     | 0.43              |
| 35:BA:2723:C:C5'   | 50:BR:2:ARG:HH11   | 2.21                     | 0.43              |
| 50:BR:48:VAL:HG12  | 50:BR:52:ILE:HG12  | 2.01                     | 0.43              |
| 51:BS:98:VAL:HG12  | 51:BS:100:ALA:CB   | 2.47                     | 0.43              |
| 52:BT:53:ARG:O     | 52:BT:59:THR:HB    | 2.18                     | 0.43              |
| 53:BU:15:LYS:HA    | 53:BU:18:LEU:HD12  | 2.00                     | 0.43              |
| 54:BV:17:GLY:O     | 54:BV:18:LEU:HB3   | 2.17                     | 0.43              |
| 58:BZ:129:SER:O    | 58:BZ:131:ARG:N    | 2.51                     | 0.43              |
| 1:CA:1055:A:C6     | 1:CA:1206:G:C5     | 3.06                     | 0.43              |
| 1:CA:1347:G:C2'    | 1:CA:1348:U:OP2    | 2.66                     | 0.43              |
| 1:CA:452:A:H5'     | 16:CP:72:ARG:NH2   | 2.33                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:CB:17:PHE:O     | 2:CB:18:GLY:C      | 2.56                     | 0.43              |
| 1:CA:1103:C:H5''  | 2:CB:98:LEU:HD13   | 1.99                     | 0.43              |
| 3:CC:101:LEU:HD23 | 3:CC:102:ASN:N     | 2.33                     | 0.43              |
| 3:CC:10:PHE:CZ    | 3:CC:178:LEU:HD11  | 2.52                     | 0.43              |
| 3:CC:136:GLN:O    | 3:CC:138:VAL:N     | 2.51                     | 0.43              |
| 5:CE:152:ARG:HB3  | 8:CH:43:GLY:HA3    | 2.00                     | 0.43              |
| 8:CH:53:VAL:HB    | 8:CH:58:TYR:CD1    | 2.53                     | 0.43              |
| 10:CJ:30:SER:O    | 10:CJ:81:THR:HG23  | 2.18                     | 0.43              |
| 1:CA:1308:U:C5    | 13:CM:99:ARG:NH1   | 2.86                     | 0.43              |
| 1:CA:1202:G:H1'   | 14:CN:29:ARG:HD3   | 2.00                     | 0.43              |
| 16:CP:75:ARG:HH11 | 16:CP:75:ARG:HG3   | 1.83                     | 0.43              |
| 24:CY:140:ASP:OD1 | 24:CY:262:SER:HB2  | 2.17                     | 0.43              |
| 24:CY:455:GLY:O   | 24:CY:456:GLU:C    | 2.55                     | 0.43              |
| 24:CY:573:HIS:CD2 | 24:CY:576:ASP:H    | 2.34                     | 0.43              |
| 24:CY:84:THR:CG2  | 61:CY:702:FUA:H152 | 2.48                     | 0.43              |
| 26:D1:24:ALA:HB3  | 26:D1:27:GLU:OE2   | 2.18                     | 0.43              |
| 26:D1:52:ARG:HD3  | 26:D1:52:ARG:HA    | 1.76                     | 0.43              |
| 30:D5:19:ARG:HG3  | 35:DA:2046:G:H5''  | 1.99                     | 0.43              |
| 31:D6:17:LYS:O    | 31:D6:18:ARG:O     | 2.37                     | 0.43              |
| 33:D8:42:ARG:C    | 33:D8:44:LYS:H     | 2.19                     | 0.43              |
| 33:D8:5:LYS:HG2   | 35:DA:242:G:C8     | 2.53                     | 0.43              |
| 35:DA:1204:A:H2   | 35:DA:1241:A:N1    | 2.16                     | 0.43              |
| 35:DA:1325:G:OP2  | 35:DA:1616:A:H2'   | 2.18                     | 0.43              |
| 35:DA:1495:A:N3   | 35:DA:1495:A:H2'   | 2.33                     | 0.43              |
| 35:DA:1663:C:HO2' | 35:DA:1664:A:C5'   | 2.31                     | 0.43              |
| 35:DA:1680:U:O2   | 35:DA:1763:G:H3'   | 2.18                     | 0.43              |
| 35:DA:1805:U:H2'  | 35:DA:1806:C:H6    | 1.82                     | 0.43              |
| 35:DA:1932:A:H2'  | 35:DA:1933:G:O4'   | 2.18                     | 0.43              |
| 26:D1:47:GLN:OE1  | 35:DA:2091:U:H1'   | 2.18                     | 0.43              |
| 35:DA:2287:A:H2   | 35:DA:2346:A:C2    | 2.36                     | 0.43              |
| 35:DA:2466:C:C2'  | 35:DA:2467:C:H5'   | 2.48                     | 0.43              |
| 35:DA:2779:U:H1'  | 35:DA:2781:A:C6    | 2.52                     | 0.43              |
| 35:DA:572:A:H2'   | 35:DA:573:G:O4'    | 2.18                     | 0.43              |
| 39:DE:103:ASP:CG  | 39:DE:201:THR:HA   | 2.37                     | 0.43              |
| 40:DF:101:LEU:O   | 40:DF:106:ARG:NH1  | 2.50                     | 0.43              |
| 40:DF:24:LEU:CB   | 40:DF:25:PRO:HD2   | 2.38                     | 0.43              |
| 42:DH:37:VAL:HG12 | 42:DH:38:SER:H     | 1.83                     | 0.43              |
| 43:DJ:9:UNK:O     | 43:DJ:10:UNK:C     | 2.67                     | 0.43              |
| 46:DN:135:PRO:O   | 46:DN:136:GLU:C    | 2.56                     | 0.43              |
| 48:DP:113:LYS:HA  | 48:DP:129:ALA:O    | 2.19                     | 0.43              |
| 48:DP:58:THR:O    | 48:DP:61:ARG:HG3   | 2.17                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 52:DT:108:ARG:CG   | 52:DT:109:GLU:N   | 2.73                     | 0.43              |
| 52:DT:8:LYS:C      | 52:DT:10:VAL:N    | 2.72                     | 0.43              |
| 52:DT:8:LYS:O      | 52:DT:10:VAL:N    | 2.50                     | 0.43              |
| 52:DT:93:ARG:HA    | 52:DT:93:ARG:HD2  | 1.78                     | 0.43              |
| 53:DU:115:ALA:C    | 53:DU:117:GLN:H   | 2.20                     | 0.43              |
| 53:DU:12:ARG:O     | 53:DU:13:LYS:C    | 2.56                     | 0.43              |
| 53:DU:59:ARG:CG    | 53:DU:59:ARG:NH1  | 2.81                     | 0.43              |
| 53:DU:88:ILE:O     | 53:DU:90:VAL:N    | 2.50                     | 0.43              |
| 55:DW:41:LYS:C     | 55:DW:43:GLY:H    | 2.21                     | 0.43              |
| 56:DX:12:VAL:CG2   | 56:DX:13:LEU:N    | 2.54                     | 0.43              |
| 57:DY:49:VAL:HG12  | 57:DY:50:ARG:N    | 2.33                     | 0.43              |
| 58:DZ:175:VAL:HB   | 58:DZ:176:PRO:CD  | 2.48                     | 0.43              |
| 1:AA:1065:U:O2'    | 1:AA:1066:C:OP2   | 2.34                     | 0.43              |
| 1:AA:1221:G:OP1    | 1:AA:1320:C:N4    | 2.52                     | 0.43              |
| 1:AA:1291:G:H2'    | 1:AA:1292:U:C6    | 2.54                     | 0.43              |
| 1:AA:1299:A:C2     | 1:AA:1301:U:N3    | 2.86                     | 0.43              |
| 1:AA:1430:C:H2'    | 1:AA:1431:C:H6    | 1.82                     | 0.43              |
| 1:AA:407:G:H2'     | 1:AA:408:A:C8     | 2.53                     | 0.43              |
| 1:AA:946:A:N6      | 1:AA:1236:A:N6    | 2.67                     | 0.43              |
| 2:AB:233:SER:HB2   | 2:AB:234:PRO:HD3  | 1.98                     | 0.43              |
| 4:AD:14:ARG:C      | 4:AD:16:GLY:N     | 2.71                     | 0.43              |
| 6:AF:43:LEU:CD1    | 6:AF:43:LEU:H     | 2.18                     | 0.43              |
| 7:AG:47:CYS:HB3    | 7:AG:58:PRO:CB    | 2.48                     | 0.43              |
| 11:AK:33:THR:HG22  | 11:AK:39:PRO:CA   | 2.43                     | 0.43              |
| 12:AL:50:SER:O     | 12:AL:51:ALA:HB2  | 2.18                     | 0.43              |
| 13:AM:94:ARG:CZ    | 19:AS:82:GLY:N    | 2.81                     | 0.43              |
| 20:AT:18:GLN:O     | 20:AT:19:SER:C    | 2.56                     | 0.43              |
| 20:AT:26:ASN:HD22  | 20:AT:26:ASN:N    | 2.14                     | 0.43              |
| 20:AT:50:GLU:HB2   | 20:AT:100:ILE:HB  | 1.99                     | 0.43              |
| 22:AV:11:A:O2'     | 22:AV:12:G:H5'    | 2.18                     | 0.43              |
| 24:AY:207:ASP:O    | 24:AY:208:GLN:C   | 2.56                     | 0.43              |
| 24:AY:238:THR:C    | 24:AY:240:GLU:H   | 2.20                     | 0.43              |
| 24:AY:355:LEU:HD12 | 24:AY:369:LEU:CD1 | 2.34                     | 0.43              |
| 24:AY:605:ILE:HD13 | 24:AY:677:GLN:HG2 | 2.00                     | 0.43              |
| 25:B0:49:LYS:HE3   | 25:B0:80:HIS:CG   | 2.53                     | 0.43              |
| 26:B1:75:GLU:OE1   | 26:B1:75:GLU:HA   | 2.19                     | 0.43              |
| 28:B3:50:VAL:O     | 28:B3:53:LEU:N    | 2.42                     | 0.43              |
| 28:B3:59:VAL:CG1   | 28:B3:60:GLU:N    | 2.77                     | 0.43              |
| 33:B8:32:LEU:CD2   | 33:B8:32:LEU:H    | 2.31                     | 0.43              |
| 35:BA:1493:C:H4'   | 35:BA:1494:A:OP1  | 2.18                     | 0.43              |
| 35:BA:1666:G:O2'   | 35:BA:1667:G:H5'  | 2.19                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:BA:2069:G:C2'  | 35:BA:2070:G:H5'  | 2.48                     | 0.43              |
| 35:BA:216:A:H2'   | 35:BA:217:G:C8    | 2.54                     | 0.43              |
| 35:BA:2439:A:C8   | 35:BA:2586:C:H4'  | 2.54                     | 0.43              |
| 35:BA:2547:U:H2'  | 35:BA:2548:G:H8   | 1.82                     | 0.43              |
| 35:BA:2694:G:O2'  | 35:BA:2695:C:H5'  | 2.17                     | 0.43              |
| 35:BA:2849:U:O4   | 52:BT:23:ARG:NH2  | 2.51                     | 0.43              |
| 35:BA:444:C:H2'   | 35:BA:445:C:C6    | 2.54                     | 0.43              |
| 35:BA:586:A:C2    | 35:BA:1254:A:C2   | 3.06                     | 0.43              |
| 35:BA:653:A:H5'   | 35:BA:654:A:P     | 2.58                     | 0.43              |
| 35:BA:959:A:N1    | 35:BA:960:A:C2    | 2.86                     | 0.43              |
| 38:BD:26:LYS:O    | 38:BD:27:THR:CG2  | 2.65                     | 0.43              |
| 39:BE:113:PHE:CE2 | 39:BE:158:GLY:CA  | 3.01                     | 0.43              |
| 39:BE:12:THR:O    | 39:BE:23:VAL:N    | 2.44                     | 0.43              |
| 41:BG:63:ILE:C    | 41:BG:63:ILE:CD1  | 2.86                     | 0.43              |
| 42:BH:173:PRO:O   | 42:BH:174:GLY:C   | 2.57                     | 0.43              |
| 48:BP:23:PRO:HD2  | 48:BP:33:ARG:HH21 | 1.83                     | 0.43              |
| 49:BQ:37:LEU:HD12 | 49:BQ:128:LYS:HB3 | 2.00                     | 0.43              |
| 52:BT:120:ARG:O   | 52:BT:124:ASP:OD1 | 2.36                     | 0.43              |
| 52:BT:57:PHE:CD2  | 52:BT:58:ASN:N    | 2.83                     | 0.43              |
| 54:BV:4:ILE:HA    | 54:BV:12:TYR:O    | 2.17                     | 0.43              |
| 57:BY:66:PRO:O    | 57:BY:67:LEU:HB3  | 2.19                     | 0.43              |
| 35:BA:336:C:H4'   | 57:BY:7:VAL:CG2   | 2.46                     | 0.43              |
| 58:BZ:20:ARG:CB   | 58:BZ:20:ARG:NH1  | 2.82                     | 0.43              |
| 58:BZ:20:ARG:NH1  | 58:BZ:20:ARG:HB2  | 2.34                     | 0.43              |
| 1:CA:1026:G:H3'   | 1:CA:1027:C:C5'   | 2.48                     | 0.43              |
| 1:CA:1409:C:O2'   | 1:CA:1410:G:H5'   | 2.18                     | 0.43              |
| 1:CA:1518:A:C2    | 1:CA:1519:A:C2    | 3.06                     | 0.43              |
| 1:CA:36:C:H4'     | 12:CL:122:THR:O   | 2.18                     | 0.43              |
| 1:CA:703:G:O2'    | 1:CA:704:A:P      | 2.76                     | 0.43              |
| 1:CA:759:A:C2'    | 1:CA:760:G:H5'    | 2.48                     | 0.43              |
| 1:CA:802:A:H3'    | 1:CA:803:G:H8     | 1.83                     | 0.43              |
| 3:CC:54:ARG:NH1   | 3:CC:54:ARG:HG2   | 2.33                     | 0.43              |
| 4:CD:125:HIS:C    | 4:CD:126:ILE:HD12 | 2.39                     | 0.43              |
| 12:CL:7:ILE:HG22  | 12:CL:8:ASN:N     | 2.34                     | 0.43              |
| 13:CM:72:ALA:O    | 13:CM:73:GLU:C    | 2.54                     | 0.43              |
| 1:CA:1048:G:OP1   | 14:CN:4:LYS:HB2   | 2.19                     | 0.43              |
| 19:CS:6:LYS:CD    | 19:CS:6:LYS:H     | 2.30                     | 0.43              |
| 22:CW:52:C:H2'    | 22:CW:53:G:O4'    | 2.18                     | 0.43              |
| 22:CW:54:G:O2'    | 22:CW:55:5MU:H5'' | 2.18                     | 0.43              |
| 25:D0:40:GLN:HE22 | 25:D0:43:THR:C    | 2.22                     | 0.43              |
| 26:D1:69:LYS:HE2  | 26:D1:72:GLU:OE1  | 2.19                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:D2:47:ASN:O     | 27:D2:48:HIS:C    | 2.55                     | 0.43              |
| 29:D4:39:CYS:SG    | 29:D4:42:PHE:CE2  | 3.10                     | 0.43              |
| 29:D4:50:VAL:O     | 29:D4:51:ASP:CB   | 2.65                     | 0.43              |
| 29:D4:7:PRO:O      | 29:D4:8:LYS:HD2   | 2.18                     | 0.43              |
| 33:D8:53:PRO:HG2   | 33:D8:54:GLU:N    | 2.33                     | 0.43              |
| 35:DA:1493:C:O2    | 35:DA:1493:C:C2'  | 2.66                     | 0.43              |
| 35:DA:1763:G:H2'   | 35:DA:1764:G:H5'  | 2.00                     | 0.43              |
| 35:DA:1925:C:O2'   | 35:DA:1926:U:H5'  | 2.18                     | 0.43              |
| 35:DA:2116:G:N7    | 35:DA:2117:A:C4   | 2.86                     | 0.43              |
| 35:DA:2309:A:H2'   | 35:DA:2310:A:H5'' | 2.00                     | 0.43              |
| 35:DA:2464:C:O2'   | 35:DA:2465:C:H6   | 2.01                     | 0.43              |
| 35:DA:2749:A:C6    | 35:DA:2750:A:N6   | 2.87                     | 0.43              |
| 30:D5:29:THR:HG21  | 35:DA:2814:C:O2'  | 2.18                     | 0.43              |
| 39:DE:38:THR:C     | 39:DE:40:GLU:H    | 2.21                     | 0.43              |
| 39:DE:65:GLY:O     | 39:DE:67:PHE:N    | 2.52                     | 0.43              |
| 39:DE:76:ARG:O     | 39:DE:77:ILE:C    | 2.57                     | 0.43              |
| 41:DG:77:ILE:HG21  | 41:DG:80:PHE:CB   | 2.40                     | 0.43              |
| 42:DH:38:SER:C     | 42:DH:40:GLU:H    | 2.22                     | 0.43              |
| 43:DJ:35:UNK:C     | 43:DJ:37:UNK:N    | 2.80                     | 0.43              |
| 43:DJ:74:UNK:C     | 43:DJ:76:UNK:N    | 2.81                     | 0.43              |
| 46:DN:133:GLN:CG   | 46:DN:134:ARG:H   | 2.31                     | 0.43              |
| 48:DP:106:LEU:O    | 48:DP:107:LYS:HG2 | 2.18                     | 0.43              |
| 48:DP:112:LEU:HD22 | 48:DP:113:LYS:N   | 2.32                     | 0.43              |
| 50:DR:94:TYR:CD1   | 50:DR:94:TYR:N    | 2.86                     | 0.43              |
| 52:DT:12:SER:O     | 52:DT:15:VAL:HG13 | 2.18                     | 0.43              |
| 53:DU:25:TRP:CD1   | 53:DU:26:GLY:N    | 2.86                     | 0.43              |
| 53:DU:31:SER:O     | 53:DU:33:ARG:N    | 2.51                     | 0.43              |
| 54:DV:19:LYS:HG3   | 54:DV:20:LEU:N    | 2.32                     | 0.43              |
| 56:DX:71:GLY:C     | 56:DX:72:LYS:HG3  | 2.38                     | 0.43              |
| 58:DZ:9:TYR:CB     | 58:DZ:35:ARG:HH22 | 2.32                     | 0.43              |
| 1:AA:1008:C:H6     | 1:AA:1008:C:O5'   | 2.00                     | 0.43              |
| 1:AA:106:C:C2'     | 1:AA:107:G:H5'    | 2.48                     | 0.43              |
| 1:AA:1081:G:O2'    | 1:AA:1082:G:H5'   | 2.19                     | 0.43              |
| 1:AA:1277:C:C3'    | 1:AA:1277:C:C6    | 3.00                     | 0.43              |
| 1:AA:1379:G:O2'    | 1:AA:1380:U:H5'   | 2.18                     | 0.43              |
| 1:AA:1494:G:H2'    | 1:AA:1494:G:N3    | 2.33                     | 0.43              |
| 1:AA:1520:G:H2'    | 1:AA:1521:G:H8    | 1.83                     | 0.43              |
| 1:AA:221:C:H2'     | 1:AA:221:C:O2     | 2.18                     | 0.43              |
| 1:AA:345:C:H5'     | 1:AA:346:G:OP1    | 2.19                     | 0.43              |
| 1:AA:393:A:H5'     | 1:AA:483:C:O2'    | 2.18                     | 0.43              |
| 1:AA:986:A:H2'     | 1:AA:987:G:H8     | 1.83                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:AB:208:ILE:HA   | 2:AB:211:ILE:HD12 | 2.00                     | 0.43              |
| 2:AB:24:TRP:CH2   | 2:AB:26:PRO:HA    | 2.52                     | 0.43              |
| 5:AE:139:LEU:O    | 5:AE:141:GLN:N    | 2.51                     | 0.43              |
| 5:AE:51:VAL:O     | 5:AE:52:PRO:C     | 2.57                     | 0.43              |
| 7:AG:120:ILE:O    | 7:AG:124:LEU:HD12 | 2.18                     | 0.43              |
| 8:AH:53:VAL:HB    | 8:AH:58:TYR:CD1   | 2.53                     | 0.43              |
| 10:AJ:27:ALA:HA   | 10:AJ:30:SER:OG   | 2.17                     | 0.43              |
| 12:AL:105:TYR:N   | 12:AL:105:TYR:CD2 | 2.85                     | 0.43              |
| 16:AP:9:PHE:CE2   | 16:AP:18:ARG:NE   | 2.86                     | 0.43              |
| 18:AR:37:VAL:O    | 18:AR:41:LYS:N    | 2.40                     | 0.43              |
| 19:AS:10:PHE:CE2  | 19:AS:37:ARG:O    | 2.72                     | 0.43              |
| 19:AS:37:ARG:H    | 19:AS:37:ARG:HG3  | 1.38                     | 0.43              |
| 24:AY:513:LYS:N   | 24:AY:566:THR:O   | 2.51                     | 0.43              |
| 25:B0:15:ASP:OD2  | 25:B0:16:SER:N    | 2.50                     | 0.43              |
| 26:B1:52:ARG:O    | 26:B1:53:VAL:HB   | 2.18                     | 0.43              |
| 26:B1:86:SER:O    | 26:B1:87:PRO:C    | 2.56                     | 0.43              |
| 27:B2:13:ALA:HA   | 27:B2:16:LEU:HD12 | 1.99                     | 0.43              |
| 27:B2:28:LYS:HB3  | 27:B2:57:ILE:CD1  | 2.48                     | 0.43              |
| 30:B5:44:THR:CG2  | 30:B5:45:VAL:N    | 2.78                     | 0.43              |
| 33:B8:56:GLU:C    | 33:B8:58:ILE:H    | 2.22                     | 0.43              |
| 35:BA:118:A:OP2   | 35:BA:119:A:H2'   | 2.18                     | 0.43              |
| 35:BA:1416:G:N3   | 35:BA:1417:C:C4   | 2.87                     | 0.43              |
| 35:BA:1899:G:N2   | 35:BA:1902:C:C5   | 2.86                     | 0.43              |
| 35:BA:216:A:H2'   | 35:BA:217:G:H8    | 1.82                     | 0.43              |
| 35:BA:2286:A:H8   | 35:BA:2287:A:C6   | 2.37                     | 0.43              |
| 35:BA:2376:A:O2'  | 51:BS:108:GLY:HA2 | 2.17                     | 0.43              |
| 35:BA:2405:G:HO2' | 35:BA:2406:U:P    | 2.41                     | 0.43              |
| 35:BA:2489:G:C6   | 35:BA:2490:G:C6   | 3.06                     | 0.43              |
| 35:BA:2696:U:H2'  | 35:BA:2697:G:H8   | 1.83                     | 0.43              |
| 35:BA:2740:A:C6   | 35:BA:2741:A:C6   | 3.06                     | 0.43              |
| 35:BA:338:G:H2'   | 35:BA:339:U:H6    | 1.83                     | 0.43              |
| 35:BA:460:A:H2'   | 35:BA:461:C:O4'   | 2.18                     | 0.43              |
| 35:BA:606:U:C2'   | 35:BA:606:U:O2    | 2.62                     | 0.43              |
| 35:BA:611:C:H2'   | 35:BA:612:C:H6    | 1.83                     | 0.43              |
| 35:BA:619:G:H3'   | 35:BA:620:G:H21   | 1.82                     | 0.43              |
| 35:BA:812:C:H1'   | 35:BA:1250:G:N2   | 2.32                     | 0.43              |
| 35:BA:886:C:H2'   | 35:BA:887:A:O4'   | 2.19                     | 0.43              |
| 35:BA:9:U:O4      | 35:BA:2629:A:N7   | 2.51                     | 0.43              |
| 38:BD:28:GLU:OE1  | 38:BD:29:PRO:HD2  | 2.18                     | 0.43              |
| 38:BD:77:ALA:HA   | 38:BD:97:TYR:HA   | 2.00                     | 0.43              |
| 39:BE:188:VAL:O   | 39:BE:189:PRO:O   | 2.36                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:BF:110:LEU:HD13 | 40:BF:202:PHE:HE1 | 1.82                     | 0.43              |
| 40:BF:116:ASP:OD1  | 40:BF:119:ARG:NH2 | 2.47                     | 0.43              |
| 40:BF:121:GLY:C    | 40:BF:123:LEU:H   | 2.22                     | 0.43              |
| 42:BH:66:GLY:CA    | 42:BH:69:ARG:HB3  | 2.43                     | 0.43              |
| 45:BL:81:UNK:O     | 45:BL:82:UNK:O    | 2.37                     | 0.43              |
| 47:BO:119:PRO:O    | 47:BO:120:GLU:HB2 | 2.18                     | 0.43              |
| 35:BA:2393:A:H5'   | 48:BP:60:MET:O    | 2.17                     | 0.43              |
| 50:BR:9:LYS:C      | 50:BR:10:LEU:HG   | 2.39                     | 0.43              |
| 51:BS:78:LEU:HD11  | 51:BS:103:GLU:HB3 | 2.00                     | 0.43              |
| 52:BT:23:ARG:HA    | 52:BT:52:ILE:HD11 | 2.01                     | 0.43              |
| 52:BT:89:VAL:C     | 52:BT:91:ARG:H    | 2.21                     | 0.43              |
| 57:BY:12:THR:HA    | 57:BY:25:GLY:O    | 2.19                     | 0.43              |
| 58:BZ:108:PRO:HA   | 58:BZ:142:SER:HA  | 2.00                     | 0.43              |
| 58:BZ:128:VAL:HG22 | 58:BZ:129:SER:N   | 2.34                     | 0.43              |
| 58:BZ:171:ILE:HG13 | 58:BZ:172:ALA:H   | 1.81                     | 0.43              |
| 58:BZ:179:ASP:CB   | 58:BZ:182:LYS:HD2 | 2.44                     | 0.43              |
| 1:CA:1062:U:H2'    | 1:CA:1063:C:C6    | 2.53                     | 0.43              |
| 1:CA:1129:C:O2'    | 1:CA:1130:A:O5'   | 2.36                     | 0.43              |
| 1:CA:1171:G:H2'    | 1:CA:1172:C:C6    | 2.52                     | 0.43              |
| 1:CA:1237:C:H2'    | 1:CA:1336:C:C5    | 2.53                     | 0.43              |
| 1:CA:1456:G:C2'    | 1:CA:1457:G:H5'   | 2.48                     | 0.43              |
| 1:CA:32:A:C2       | 1:CA:33:A:C4      | 3.06                     | 0.43              |
| 1:CA:659:U:O2'     | 1:CA:660:G:H5'    | 2.18                     | 0.43              |
| 1:CA:773:G:C2'     | 1:CA:774:G:H5'    | 2.48                     | 0.43              |
| 2:CB:144:ARG:O     | 2:CB:145:LEU:C    | 2.57                     | 0.43              |
| 2:CB:51:LEU:HD22   | 2:CB:55:PHE:HE2   | 1.83                     | 0.43              |
| 3:CC:90:GLU:OE1    | 3:CC:93:LYS:HD2   | 2.18                     | 0.43              |
| 4:CD:134:ASP:OD2   | 4:CD:134:ASP:N    | 2.51                     | 0.43              |
| 4:CD:58:LEU:HD23   | 4:CD:62:GLN:HG2   | 2.00                     | 0.43              |
| 5:CE:80:ILE:CD1    | 5:CE:138:ALA:HB1  | 2.48                     | 0.43              |
| 7:CG:85:TYR:CD1    | 7:CG:154:TYR:HE1  | 2.36                     | 0.43              |
| 8:CH:53:VAL:HB     | 8:CH:58:TYR:CE1   | 2.54                     | 0.43              |
| 8:CH:6:ILE:O       | 8:CH:9:MET:N      | 2.51                     | 0.43              |
| 10:CJ:22:LYS:NZ    | 10:CJ:88:LEU:HD23 | 2.33                     | 0.43              |
| 11:CK:79:SER:CB    | 11:CK:106:LYS:HD2 | 2.48                     | 0.43              |
| 13:CM:36:LYS:HG3   | 13:CM:59:TYR:OH   | 2.19                     | 0.43              |
| 14:CN:48:ALA:CA    | 14:CN:53:LEU:HD12 | 2.49                     | 0.43              |
| 16:CP:20:VAL:HG22  | 16:CP:21:VAL:N    | 2.33                     | 0.43              |
| 18:CR:58:LEU:CD1   | 18:CR:58:LEU:N    | 2.81                     | 0.43              |
| 19:CS:29:ARG:HD2   | 19:CS:29:ARG:N    | 2.32                     | 0.43              |
| 24:CY:415:PRO:HG3  | 24:CY:421:GLN:HG2 | 2.01                     | 0.43              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:D0:12:ASN:C     | 25:D0:14:ARG:H     | 2.21                     | 0.43              |
| 29:D4:2:LYS:HG2    | 36:DB:44:G:P       | 2.58                     | 0.43              |
| 19:CS:9:VAL:CG2    | 29:D4:53:GLU:OE2   | 2.66                     | 0.43              |
| 32:D7:34:ARG:HH12  | 32:D7:39:ARG:CD    | 2.32                     | 0.43              |
| 34:D9:11:CYS:SG    | 34:D9:11:CYS:O     | 2.76                     | 0.43              |
| 34:D9:34:GLN:O     | 34:D9:35:ARG:CB    | 2.66                     | 0.43              |
| 35:DA:1115:G:C8    | 35:DA:1115:G:H5'   | 2.49                     | 0.43              |
| 35:DA:1161:C:H2'   | 35:DA:1162:G:C8    | 2.54                     | 0.43              |
| 35:DA:1319:G:C2    | 35:DA:1334:G:C6    | 3.06                     | 0.43              |
| 35:DA:1342:A:C2    | 35:DA:1345:C:C5    | 3.07                     | 0.43              |
| 35:DA:1782:C:C2'   | 35:DA:1783:A:H5'   | 2.47                     | 0.43              |
| 35:DA:1819:A:O2'   | 35:DA:1820:U:P     | 2.76                     | 0.43              |
| 35:DA:1902:C:H4'   | 38:DD:244:ARG:CB   | 2.46                     | 0.43              |
| 35:DA:2081:C:H2'   | 35:DA:2082:A:C8    | 2.54                     | 0.43              |
| 35:DA:2140:C:H1'   | 35:DA:2152:G:N2    | 2.34                     | 0.43              |
| 35:DA:2219:G:C2'   | 35:DA:2220:G:H5'   | 2.49                     | 0.43              |
| 35:DA:268:C:H2'    | 35:DA:268:C:O2     | 2.17                     | 0.43              |
| 35:DA:2704:C:O2'   | 35:DA:2705:A:H5'   | 2.19                     | 0.43              |
| 35:DA:492:A:H2'    | 35:DA:493:G:C5'    | 2.49                     | 0.43              |
| 35:DA:625:G:H5'    | 35:DA:657:U:OP1    | 2.19                     | 0.43              |
| 38:DD:270:ILE:N    | 38:DD:270:ILE:HD12 | 2.34                     | 0.43              |
| 39:DE:167:VAL:HG22 | 39:DE:170:LEU:HD11 | 2.00                     | 0.43              |
| 40:DF:68:LYS:HG3   | 40:DF:69:HIS:CD2   | 2.54                     | 0.43              |
| 41:DG:64:THR:HG23  | 41:DG:65:GLY:N     | 2.33                     | 0.43              |
| 45:DL:76:UNK:O     | 45:DL:80:UNK:N     | 2.51                     | 0.43              |
| 46:DN:119:ARG:HG3  | 46:DN:119:ARG:NH1  | 2.33                     | 0.43              |
| 1:CA:1423:G:H5'    | 47:DO:49:ARG:HH22  | 1.82                     | 0.43              |
| 48:DP:107:LYS:O    | 48:DP:109:GLY:N    | 2.51                     | 0.43              |
| 35:DA:661:C:O2'    | 48:DP:16:ARG:O     | 2.32                     | 0.43              |
| 48:DP:25:SER:O     | 48:DP:30:THR:CG2   | 2.65                     | 0.43              |
| 49:DQ:137:TYR:N    | 49:DQ:137:TYR:CD1  | 2.84                     | 0.43              |
| 51:DS:36:TYR:HD1   | 51:DS:36:TYR:N     | 2.14                     | 0.43              |
| 52:DT:29:ARG:O     | 52:DT:30:VAL:O     | 2.36                     | 0.43              |
| 54:DV:17:GLY:O     | 54:DV:18:LEU:HB3   | 2.18                     | 0.43              |
| 57:DY:61:ILE:CG1   | 57:DY:62:GLU:N     | 2.80                     | 0.43              |
| 57:DY:84:ARG:HD2   | 57:DY:97:ARG:HD2   | 2.01                     | 0.43              |
| 58:DZ:61:LEU:HB2   | 58:DZ:65:GLN:HB2   | 2.00                     | 0.43              |
| 1:AA:1202:G:H1'    | 14:AN:29:ARG:HD3   | 2.01                     | 0.43              |
| 1:AA:64:G:N2       | 1:AA:67:C:C4       | 2.86                     | 0.43              |
| 1:AA:748:C:O2'     | 1:AA:749:C:O5'     | 2.36                     | 0.43              |
| 1:AA:757:U:O2'     | 1:AA:879:C:H1'     | 2.18                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:AD:86:LYS:HD3    | 4:AD:86:LYS:HA     | 1.82                     | 0.43              |
| 5:AE:80:ILE:CD1    | 5:AE:138:ALA:HB1   | 2.49                     | 0.43              |
| 6:AF:67:MET:CE     | 6:AF:75:LEU:HD22   | 2.48                     | 0.43              |
| 14:AN:12:ARG:NH1   | 14:AN:12:ARG:HB2   | 2.34                     | 0.43              |
| 14:AN:21:TYR:OH    | 14:AN:23:ARG:NH2   | 2.50                     | 0.43              |
| 17:AQ:33:GLY:O     | 17:AQ:34:LYS:C     | 2.56                     | 0.43              |
| 18:AR:87:ARG:CZ    | 18:AR:87:ARG:HB3   | 2.48                     | 0.43              |
| 13:AM:91:ARG:NH2   | 19:AS:81:ARG:NH2   | 2.66                     | 0.43              |
| 22:AV:14:A:H1'     | 22:AV:22:G:N2      | 2.33                     | 0.43              |
| 24:AY:165:GLN:HA   | 24:AY:178:ILE:O    | 2.19                     | 0.43              |
| 24:AY:170:ARG:HD2  | 24:AY:170:ARG:H    | 1.84                     | 0.43              |
| 24:AY:187:THR:OG1  | 24:AY:188:TYR:N    | 2.52                     | 0.43              |
| 24:AY:485:GLU:HB2  | 24:AY:560:VAL:HA   | 1.99                     | 0.43              |
| 24:AY:409:ILE:HG12 | 24:AY:656:ALA:CB   | 2.49                     | 0.43              |
| 24:AY:519:ARG:HD3  | 24:AY:677:GLN:HA   | 2.01                     | 0.43              |
| 24:AY:601:ILE:O    | 24:AY:679:VAL:HG13 | 2.19                     | 0.43              |
| 27:B2:14:ARG:NH1   | 27:B2:14:ARG:HG3   | 2.33                     | 0.43              |
| 28:B3:19:GLN:O     | 28:B3:22:ALA:N     | 2.43                     | 0.43              |
| 29:B4:30:GLU:C     | 29:B4:31:ILE:HD12  | 2.38                     | 0.43              |
| 35:BA:1144:G:C6    | 35:BA:1145:C:C4    | 3.06                     | 0.43              |
| 35:BA:1314:C:H5'   | 35:BA:1314:C:C6    | 2.37                     | 0.43              |
| 35:BA:1385:G:H1'   | 35:BA:1386:C:C6    | 2.53                     | 0.43              |
| 35:BA:1452:A:H3'   | 35:BA:1453:U:H5'   | 1.91                     | 0.43              |
| 35:BA:1565:C:C2    | 35:BA:1567:A:C8    | 3.06                     | 0.43              |
| 35:BA:1575:C:O2    | 35:BA:1575:C:H2'   | 2.17                     | 0.43              |
| 35:BA:1675:C:H2'   | 35:BA:1676:A:O4'   | 2.19                     | 0.43              |
| 35:BA:1999:C:O2'   | 35:BA:2000:G:H5'   | 2.19                     | 0.43              |
| 35:BA:2296:U:C4'   | 35:BA:2297:C:OP1   | 2.54                     | 0.43              |
| 35:BA:2308:G:N7    | 35:BA:2310:A:C5'   | 2.70                     | 0.43              |
| 35:BA:2749:A:C6    | 35:BA:2750:A:N6    | 2.86                     | 0.43              |
| 35:BA:294:A:H2'    | 35:BA:295:G:H5'    | 1.99                     | 0.43              |
| 35:BA:476:G:H4'    | 35:BA:502:A:N1     | 2.33                     | 0.43              |
| 35:BA:558:G:P      | 46:BN:111:PRO:HD2  | 2.57                     | 0.43              |
| 35:BA:677:A:O2'    | 35:BA:678:C:H5'    | 2.19                     | 0.43              |
| 36:BB:106:G:O2'    | 36:BB:107:G:H5'    | 2.18                     | 0.43              |
| 36:BB:82:G:C2      | 36:BB:83:G:C8      | 3.07                     | 0.43              |
| 37:BC:46:ALA:HA    | 37:BC:212:SER:O    | 2.18                     | 0.43              |
| 38:BD:127:VAL:HG22 | 38:BD:194:GLY:HA3  | 2.01                     | 0.43              |
| 38:BD:213:ARG:HD2  | 38:BD:213:ARG:HA   | 1.74                     | 0.43              |
| 39:BE:108:SER:O    | 39:BE:109:LYS:C    | 2.55                     | 0.43              |
| 39:BE:1:MET:O      | 39:BE:2:LYS:C      | 2.56                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 39:BE:21:VAL:HG23 | 39:BE:21:VAL:O     | 2.19                     | 0.43              |
| 39:BE:38:THR:OG1  | 39:BE:41:LYS:HE2   | 2.18                     | 0.43              |
| 39:BE:31:CYS:HB3  | 39:BE:49:LEU:HB3   | 2.01                     | 0.43              |
| 40:BF:192:LEU:C   | 40:BF:192:LEU:CD2  | 2.87                     | 0.43              |
| 42:BH:105:LEU:CD2 | 42:BH:105:LEU:N    | 2.82                     | 0.43              |
| 47:BO:61:VAL:O    | 47:BO:84:ALA:HA    | 2.17                     | 0.43              |
| 49:BQ:132:VAL:HB  | 49:BQ:137:TYR:OH   | 2.18                     | 0.43              |
| 50:BR:12:ARG:HD3  | 50:BR:16:HIS:CD2   | 2.53                     | 0.43              |
| 39:BE:111:ARG:CZ  | 50:BR:2:ARG:NH2    | 2.81                     | 0.43              |
| 51:BS:74:ALA:HB2  | 51:BS:101:LEU:HD22 | 2.00                     | 0.43              |
| 52:BT:8:LYS:C     | 52:BT:10:VAL:N     | 2.71                     | 0.43              |
| 54:BV:5:VAL:HG22  | 54:BV:6:LYS:N      | 2.34                     | 0.43              |
| 55:BW:44:ALA:O    | 55:BW:45:TYR:C     | 2.57                     | 0.43              |
| 56:BX:10:ALA:O    | 56:BX:28:PHE:CB    | 2.64                     | 0.43              |
| 58:BZ:50:GLN:O    | 58:BZ:51:ALA:C     | 2.57                     | 0.43              |
| 1:CA:115:G:H1'    | 1:CA:116:A:N7      | 2.33                     | 0.43              |
| 1:CA:1174:G:O2'   | 1:CA:1175:G:H5'    | 2.19                     | 0.43              |
| 1:CA:1347:G:H2'   | 1:CA:1373:G:O6     | 2.18                     | 0.43              |
| 1:CA:1392:G:O2'   | 1:CA:1393:U:H5'    | 2.18                     | 0.43              |
| 1:CA:1443:G:C6    | 1:CA:1460:A:C2     | 3.06                     | 0.43              |
| 1:CA:182:U:O2     | 1:CA:182:U:H2'     | 2.18                     | 0.43              |
| 1:CA:142:G:N3     | 1:CA:196:A:H2      | 2.17                     | 0.43              |
| 1:CA:502:G:OP1    | 12:CL:118:SER:N    | 2.39                     | 0.43              |
| 1:CA:596:C:H6     | 1:CA:596:C:O5'     | 2.02                     | 0.43              |
| 1:CA:757:U:H2'    | 1:CA:758:G:O4'     | 2.19                     | 0.43              |
| 1:CA:977:A:N3     | 1:CA:977:A:H3'     | 2.34                     | 0.43              |
| 2:CB:44:LEU:N     | 2:CB:44:LEU:HD12   | 2.15                     | 0.43              |
| 3:CC:129:ALA:O    | 3:CC:131:ARG:N     | 2.52                     | 0.43              |
| 3:CC:79:ARG:NH1   | 3:CC:79:ARG:HB2    | 2.14                     | 0.43              |
| 4:CD:159:ARG:O    | 4:CD:162:LEU:N     | 2.52                     | 0.43              |
| 5:CE:72:GLN:NE2   | 5:CE:144:THR:HG22  | 2.32                     | 0.43              |
| 6:CF:53:ALA:C     | 6:CF:55:ASP:H      | 2.21                     | 0.43              |
| 1:CA:1375:A:OP1   | 7:CG:12:LEU:HD21   | 2.18                     | 0.43              |
| 8:CH:104:ARG:O    | 8:CH:107:LEU:N     | 2.51                     | 0.43              |
| 8:CH:30:ARG:HH11  | 8:CH:30:ARG:HB2    | 1.82                     | 0.43              |
| 10:CJ:63:PHE:HB2  | 14:CN:57:ARG:O     | 2.19                     | 0.43              |
| 10:CJ:78:ASN:C    | 10:CJ:79:ARG:NH1   | 2.71                     | 0.43              |
| 11:CK:126:ARG:O   | 11:CK:127:LYS:C    | 2.56                     | 0.43              |
| 1:CA:34:C:H1'     | 12:CL:32:PHE:CZ    | 2.53                     | 0.43              |
| 1:CA:1115:C:H1'   | 14:CN:61:TRP:O     | 2.18                     | 0.43              |
| 16:CP:6:LEU:HG    | 16:CP:17:TYR:HB3   | 2.01                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 20:CT:49:ALA:HB3  | 20:CT:99:LEU:CD1   | 2.48                     | 0.43              |
| 26:D1:4:VAL:HG23  | 26:D1:9:GLY:O      | 2.19                     | 0.43              |
| 27:D2:14:ARG:HG3  | 27:D2:14:ARG:NH1   | 2.33                     | 0.43              |
| 27:D2:48:HIS:O    | 27:D2:50:ILE:N     | 2.51                     | 0.43              |
| 27:D2:62:THR:O    | 27:D2:65:ASN:HB2   | 2.18                     | 0.43              |
| 30:D5:4:HIS:CB    | 30:D5:5:PRO:CD     | 2.92                     | 0.43              |
| 31:D6:15:GLU:OE1  | 31:D6:41:PRO:HG3   | 2.19                     | 0.43              |
| 32:D7:27:GLY:HA2  | 32:D7:30:VAL:CG2   | 2.49                     | 0.43              |
| 35:DA:1230:C:H2'  | 35:DA:1231:G:H8    | 1.83                     | 0.43              |
| 35:DA:1314:C:OP1  | 35:DA:1315:C:OP2   | 2.36                     | 0.43              |
| 35:DA:1416:G:N3   | 35:DA:1417:C:C4    | 2.87                     | 0.43              |
| 35:DA:1638:C:O2'  | 35:DA:1639:U:H5'   | 2.18                     | 0.43              |
| 35:DA:1326:U:H4'  | 35:DA:2011:U:O4'   | 2.19                     | 0.43              |
| 35:DA:2552:U:H2'  | 35:DA:2554:U:H5"   | 2.00                     | 0.43              |
| 38:DD:45:ASN:HB2  | 38:DD:46:GLN:OE1   | 2.18                     | 0.43              |
| 38:DD:73:VAL:C    | 38:DD:75:ILE:H     | 2.22                     | 0.43              |
| 39:DE:27:LEU:HD12 | 39:DE:181:LEU:HD13 | 1.99                     | 0.43              |
| 39:DE:36:ARG:NH1  | 39:DE:85:ASN:OD1   | 2.49                     | 0.43              |
| 40:DF:187:VAL:CG1 | 48:DP:7:ARG:HH22   | 2.31                     | 0.43              |
| 41:DG:139:LEU:C   | 41:DG:141:PHE:H    | 2.22                     | 0.43              |
| 41:DG:141:PHE:CB  | 41:DG:144:ILE:HG22 | 2.46                     | 0.43              |
| 41:DG:163:ALA:HB1 | 41:DG:168:GLU:HB2  | 1.99                     | 0.43              |
| 41:DG:45:GLU:OE2  | 41:DG:45:GLU:CA    | 2.65                     | 0.43              |
| 41:DG:76:SER:HB3  | 41:DG:83:ARG:HB3   | 1.98                     | 0.43              |
| 42:DH:154:PRO:HB2 | 42:DH:155:SER:H    | 1.59                     | 0.43              |
| 42:DH:35:VAL:CG2  | 42:DH:75:ALA:HB2   | 2.49                     | 0.43              |
| 47:DO:87:ILE:HG22 | 47:DO:92:GLU:C     | 2.38                     | 0.43              |
| 35:DA:943:U:OP2   | 48:DP:38:GLN:CD    | 2.56                     | 0.43              |
| 49:DQ:56:ARG:CA   | 49:DQ:56:ARG:NE    | 2.77                     | 0.43              |
| 50:DR:41:ALA:C    | 50:DR:43:GLU:N     | 2.70                     | 0.43              |
| 50:DR:63:ARG:O    | 50:DR:67:LEU:HD23  | 2.19                     | 0.43              |
| 51:DS:101:LEU:C   | 51:DS:101:LEU:CD1  | 2.87                     | 0.43              |
| 52:DT:11:GLU:C    | 52:DT:13:ARG:N     | 2.70                     | 0.43              |
| 54:DV:5:VAL:HG22  | 54:DV:6:LYS:N      | 2.33                     | 0.43              |
| 35:DA:1614:A:H62  | 55:DW:93:ALA:HB2   | 1.83                     | 0.43              |
| 56:DX:10:ALA:O    | 56:DX:28:PHE:CB    | 2.66                     | 0.43              |
| 1:AA:1000:U:H3'   | 1:AA:1000:U:H6     | 1.84                     | 0.43              |
| 1:AA:1422:G:C2    | 1:AA:1423:G:C5     | 3.07                     | 0.43              |
| 1:AA:1457:G:O5'   | 1:AA:1457:G:H8     | 2.01                     | 0.43              |
| 1:AA:186:C:C2     | 1:AA:187:C:C5      | 3.06                     | 0.43              |
| 1:AA:67:C:H2'     | 1:AA:68:G:H8       | 1.83                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:697:U:H2'     | 1:AA:698:G:C5'     | 2.38                     | 0.43              |
| 2:AB:12:GLU:OE1    | 2:AB:12:GLU:N      | 2.39                     | 0.43              |
| 2:AB:142:LEU:O     | 2:AB:146:GLN:HB2   | 2.19                     | 0.43              |
| 2:AB:178:ARG:CB    | 2:AB:178:ARG:HH11  | 2.31                     | 0.43              |
| 3:AC:105:GLU:HG2   | 3:AC:106:VAL:N     | 2.30                     | 0.43              |
| 4:AD:73:ARG:HD3    | 4:AD:73:ARG:HA     | 1.79                     | 0.43              |
| 4:AD:9:CYS:SG      | 4:AD:22:LYS:HD2    | 2.59                     | 0.43              |
| 5:AE:119:LEU:N     | 5:AE:119:LEU:HD23  | 2.34                     | 0.43              |
| 7:AG:22:LEU:HD23   | 7:AG:22:LEU:O      | 2.19                     | 0.43              |
| 8:AH:38:ILE:O      | 8:AH:39:LEU:C      | 2.57                     | 0.43              |
| 8:AH:46:LYS:HG3    | 8:AH:64:LYS:HB2    | 1.99                     | 0.43              |
| 13:AM:29:ARG:HB3   | 13:AM:64:TRP:CZ2   | 2.54                     | 0.43              |
| 13:AM:3:ARG:CA     | 13:AM:9:ILE:HG13   | 2.45                     | 0.43              |
| 1:AA:1316:G:O3'    | 14:AN:18:VAL:CG1   | 2.66                     | 0.43              |
| 14:AN:47:LEU:O     | 14:AN:48:ALA:C     | 2.56                     | 0.43              |
| 1:AA:235:C:C5'     | 17:AQ:70:ARG:HG2   | 2.45                     | 0.43              |
| 17:AQ:67:LYS:CA    | 17:AQ:70:ARG:HH12  | 2.25                     | 0.43              |
| 17:AQ:88:TYR:O     | 17:AQ:89:LEU:C     | 2.57                     | 0.43              |
| 20:AT:86:ARG:HG3   | 20:AT:86:ARG:NH1   | 2.33                     | 0.43              |
| 24:AY:484:ARG:HA   | 24:AY:484:ARG:HD3  | 1.60                     | 0.43              |
| 24:AY:487:ILE:CD1  | 24:AY:487:ILE:N    | 2.81                     | 0.43              |
| 26:B1:82:LEU:HD12  | 26:B1:82:LEU:N     | 2.33                     | 0.43              |
| 13:AM:57:ARG:HH12  | 29:B4:34:GLU:HG3   | 1.83                     | 0.43              |
| 33:B8:42:ARG:C     | 33:B8:44:LYS:H     | 2.17                     | 0.43              |
| 35:BA:1432:C:H2'   | 35:BA:1433:U:C6    | 2.54                     | 0.43              |
| 35:BA:2081:C:H2'   | 35:BA:2082:A:C8    | 2.53                     | 0.43              |
| 35:BA:2154:G:H2'   | 35:BA:2155:G:H8    | 1.83                     | 0.43              |
| 35:BA:2287:A:N6    | 35:BA:2344:U:C2    | 2.86                     | 0.43              |
| 35:BA:2701:C:H2'   | 35:BA:2702:U:H2'   | 2.00                     | 0.43              |
| 35:BA:27:G:C2'     | 35:BA:28:A:OP2     | 2.66                     | 0.43              |
| 35:BA:654(B):C:H2' | 35:BA:654(C):G:C8  | 2.53                     | 0.43              |
| 35:BA:854:G:H1     | 35:BA:923:C:H42    | 1.67                     | 0.43              |
| 35:BA:978:G:N2     | 35:BA:979:G:H1'    | 2.33                     | 0.43              |
| 36:BB:67:G:O2'     | 36:BB:68:C:H5'     | 2.18                     | 0.43              |
| 38:BD:142:VAL:HG23 | 38:BD:192:THR:O    | 2.18                     | 0.43              |
| 39:BE:15:PHE:CZ    | 52:BT:80:SER:HB2   | 2.53                     | 0.43              |
| 39:BE:93:VAL:HG12  | 39:BE:175:VAL:CG2  | 2.48                     | 0.43              |
| 39:BE:1:MET:O      | 39:BE:2:LYS:O      | 2.36                     | 0.43              |
| 39:BE:76:ARG:O     | 39:BE:77:ILE:C     | 2.56                     | 0.43              |
| 40:BF:8:GLN:HG2    | 40:BF:126:VAL:HG12 | 2.01                     | 0.43              |
| 40:BF:84:VAL:CG1   | 40:BF:85:GLY:N     | 2.55                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:BG:149:VAL:O    | 41:BG:149:VAL:HG13 | 2.19                     | 0.43              |
| 42:BH:35:VAL:HG21  | 42:BH:75:ALA:HB2   | 2.00                     | 0.43              |
| 46:BN:13:TRP:O     | 46:BN:135:PRO:HD2  | 2.19                     | 0.43              |
| 46:BN:24:GLY:CA    | 46:BN:27:ALA:HB3   | 2.49                     | 0.43              |
| 46:BN:40:PRO:HB3   | 53:BU:68:ALA:HB2   | 2.01                     | 0.43              |
| 46:BN:57:ALA:HB3   | 46:BN:124:ALA:HA   | 2.00                     | 0.43              |
| 50:BR:24:GLN:NE2   | 50:BR:36:THR:HG21  | 2.34                     | 0.43              |
| 51:BS:28:VAL:HG13  | 51:BS:36:TYR:O     | 2.18                     | 0.43              |
| 52:BT:32:TYR:O     | 52:BT:33:LYS:HB2   | 2.19                     | 0.43              |
| 55:BW:17:VAL:O     | 55:BW:19:LEU:N     | 2.51                     | 0.43              |
| 55:BW:62:HIS:O     | 55:BW:63:ASP:C     | 2.56                     | 0.43              |
| 1:CA:1442(B):A:C2  | 52:DT:118:ARG:NH2  | 2.87                     | 0.43              |
| 1:CA:514:C:H2'     | 1:CA:515:G:H8      | 1.82                     | 0.43              |
| 2:CB:21:ARG:HB3    | 2:CB:39:ILE:HG12   | 2.00                     | 0.43              |
| 2:CB:55:PHE:HE1    | 2:CB:218:ALA:HA    | 1.83                     | 0.43              |
| 2:CB:70:PHE:O      | 2:CB:92:TYR:HA     | 2.17                     | 0.43              |
| 3:CC:139:GLN:O     | 3:CC:140:ARG:C     | 2.57                     | 0.43              |
| 3:CC:3:ASN:N       | 3:CC:3:ASN:OD1     | 2.51                     | 0.43              |
| 4:CD:54:TYR:O      | 4:CD:55:ALA:C      | 2.57                     | 0.43              |
| 5:CE:11:ILE:HD12   | 5:CE:31:LEU:HD13   | 2.01                     | 0.43              |
| 5:CE:12:LEU:HD12   | 5:CE:12:LEU:H      | 1.82                     | 0.43              |
| 7:CG:120:ILE:O     | 7:CG:124:LEU:HB2   | 2.19                     | 0.43              |
| 7:CG:50:ILE:O      | 7:CG:54:THR:HG23   | 2.19                     | 0.43              |
| 10:CJ:3:LYS:HZ3    | 10:CJ:77:PRO:HD2   | 1.82                     | 0.43              |
| 11:CK:60:ALA:O     | 11:CK:61:ALA:C     | 2.56                     | 0.43              |
| 13:CM:35:GLU:CG    | 13:CM:36:LYS:N     | 2.82                     | 0.43              |
| 13:CM:46:LYS:O     | 13:CM:46:LYS:HD3   | 2.19                     | 0.43              |
| 13:CM:79:LYS:HA    | 13:CM:82:MET:CG    | 2.48                     | 0.43              |
| 17:CQ:9:VAL:CG1    | 17:CQ:56:VAL:HG22  | 2.48                     | 0.43              |
| 18:CR:87:ARG:HB3   | 18:CR:87:ARG:CZ    | 2.48                     | 0.43              |
| 19:CS:64:GLU:HG2   | 29:D4:48:ARG:HH21  | 1.79                     | 0.43              |
| 20:CT:81:LYS:C     | 20:CT:83:ARG:N     | 2.72                     | 0.43              |
| 22:CW:55:5MU:H2'   | 22:CW:56:U:O4'     | 2.18                     | 0.43              |
| 24:CY:630:GLN:HE22 | 24:CY:646:PHE:HB2  | 1.84                     | 0.43              |
| 24:CY:688:ILE:N    | 24:CY:688:ILE:HD12 | 2.33                     | 0.43              |
| 24:CY:71:THR:HG21  | 24:CY:357:ARG:CD   | 2.47                     | 0.43              |
| 24:CY:85:PRO:HA    | 24:CY:94:VAL:HG22  | 2.00                     | 0.43              |
| 27:D2:40:SER:O     | 27:D2:42:GLY:N     | 2.51                     | 0.43              |
| 28:D3:31:LEU:HD12  | 35:DA:1157:G:O2'   | 2.18                     | 0.43              |
| 19:CS:43:GLU:OE1   | 29:D4:56:VAL:HG22  | 2.18                     | 0.43              |
| 32:D7:46:VAL:CG1   | 32:D7:47:ARG:H     | 2.32                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:D7:8:ASN:C     | 32:D7:8:ASN:HD22   | 2.19                     | 0.43              |
| 34:D9:29:ASN:N    | 34:D9:29:ASN:HD22  | 2.17                     | 0.43              |
| 35:DA:1541:G:H5'' | 35:DA:1542:A:OP1   | 2.17                     | 0.43              |
| 35:DA:1668:A:H4'  | 35:DA:1669:A:O5'   | 2.19                     | 0.43              |
| 35:DA:1693:U:O2'  | 38:DD:14:ARG:NH2   | 2.51                     | 0.43              |
| 35:DA:2009:G:O2'  | 35:DA:2010:G:H5'   | 2.19                     | 0.43              |
| 35:DA:2400:G:N2   | 35:DA:2417:C:C2    | 2.87                     | 0.43              |
| 35:DA:245:G:O2'   | 35:DA:246:C:H5'    | 2.19                     | 0.43              |
| 35:DA:2841:C:O2'  | 35:DA:2842:G:H5'   | 2.19                     | 0.43              |
| 35:DA:332:A:O2'   | 35:DA:334:C:OP2    | 2.35                     | 0.43              |
| 35:DA:445:C:O2    | 35:DA:449:A:H2     | 2.01                     | 0.43              |
| 35:DA:520:G:H2'   | 35:DA:521:G:C8     | 2.52                     | 0.43              |
| 37:DC:73:VAL:O    | 37:DC:73:VAL:HG13  | 2.18                     | 0.43              |
| 37:DC:90:ALA:HA   | 37:DC:155:ARG:HH12 | 1.79                     | 0.43              |
| 38:DD:92:ILE:H    | 38:DD:92:ILE:HD13  | 1.82                     | 0.43              |
| 40:DF:29:ASN:O    | 40:DF:30:PRO:C     | 2.56                     | 0.43              |
| 41:DG:125:PHE:CE1 | 41:DG:170:ARG:HD2  | 2.53                     | 0.43              |
| 41:DG:11:TYR:OH   | 41:DG:33:ARG:CG    | 2.67                     | 0.43              |
| 41:DG:55:LYS:HD3  | 41:DG:56:ALA:CA    | 2.47                     | 0.43              |
| 41:DG:67:LYS:HD3  | 41:DG:68:PRO:O     | 2.19                     | 0.43              |
| 43:DJ:108:UNK:O   | 43:DJ:109:UNK:C    | 2.65                     | 0.43              |
| 48:DP:107:LYS:HB2 | 48:DP:107:LYS:HE3  | 1.79                     | 0.43              |
| 48:DP:12:ALA:CB   | 48:DP:16:ARG:HB3   | 2.49                     | 0.43              |
| 35:DA:2376:A:O2'  | 51:DS:108:GLY:HA2  | 2.18                     | 0.43              |
| 52:DT:90:GLN:O    | 52:DT:92:GLY:N     | 2.51                     | 0.43              |
| 53:DU:5:LYS:HB2   | 53:DU:5:LYS:HE3    | 1.86                     | 0.43              |
| 53:DU:91:ASP:O    | 53:DU:92:ARG:HB3   | 2.19                     | 0.43              |
| 55:DW:66:GLU:HG3  | 55:DW:69:LEU:HD12  | 1.99                     | 0.43              |
| 58:DZ:39:VAL:O    | 58:DZ:39:VAL:HG23  | 2.19                     | 0.43              |
| 1:AA:323:U:H2'    | 1:AA:324:G:O4'     | 2.19                     | 0.43              |
| 1:AA:608:A:O2'    | 1:AA:609:A:H5'     | 2.19                     | 0.43              |
| 1:AA:636:U:H2'    | 1:AA:637:G:H8      | 1.83                     | 0.43              |
| 1:AA:743:U:H2'    | 1:AA:744:C:C6      | 2.53                     | 0.43              |
| 3:AC:129:ALA:O    | 3:AC:131:ARG:N     | 2.51                     | 0.43              |
| 3:AC:129:ALA:C    | 3:AC:131:ARG:N     | 2.72                     | 0.43              |
| 3:AC:32:LEU:HD22  | 3:AC:59:ARG:HH12   | 1.83                     | 0.43              |
| 4:AD:18:LYS:HE2   | 4:AD:20:TYR:CE2    | 2.53                     | 0.43              |
| 7:AG:129:GLU:OE2  | 7:AG:131:LYS:HE2   | 2.18                     | 0.43              |
| 7:AG:144:MET:O    | 7:AG:147:ALA:HB3   | 2.19                     | 0.43              |
| 10:AJ:30:SER:O    | 10:AJ:81:THR:HG23  | 2.18                     | 0.43              |
| 15:AO:48:LYS:HD3  | 15:AO:48:LYS:HA    | 1.72                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:AP:27:LYS:HG2   | 16:AP:30:GLY:HA3   | 2.00                     | 0.43              |
| 19:AS:15:LEU:HD13  | 19:AS:31:ILE:HD11  | 2.01                     | 0.43              |
| 21:AU:6:ARG:NH2    | 21:AU:15:ARG:HH22  | 2.17                     | 0.43              |
| 22:AV:29:G:O2'     | 22:AV:30:G:H5'     | 2.19                     | 0.43              |
| 24:AY:228:MET:CE   | 24:AY:229:LEU:HG   | 2.48                     | 0.43              |
| 24:AY:260:LEU:N    | 24:AY:260:LEU:HD13 | 2.33                     | 0.43              |
| 24:AY:525:PHE:HA   | 24:AY:565:VAL:O    | 2.19                     | 0.43              |
| 24:AY:519:ARG:HH12 | 24:AY:678:GLU:CB   | 2.32                     | 0.43              |
| 25:B0:37:LEU:HG    | 25:B0:60:PHE:HA    | 2.01                     | 0.43              |
| 25:B0:40:GLN:HE22  | 25:B0:43:THR:C     | 2.22                     | 0.43              |
| 27:B2:38:GLN:HA    | 27:B2:41:ILE:HG12  | 2.01                     | 0.43              |
| 27:B2:59:ARG:HG2   | 27:B2:59:ARG:H     | 1.47                     | 0.43              |
| 29:B4:31:ILE:HG23  | 29:B4:33:VAL:HG23  | 2.00                     | 0.43              |
| 33:B8:61:LEU:N     | 33:B8:63:PRO:HD2   | 2.34                     | 0.43              |
| 34:B9:16:VAL:O     | 35:BA:1033:U:H5    | 2.00                     | 0.43              |
| 35:BA:1310:G:C2'   | 35:BA:1311:G:H5'   | 2.49                     | 0.43              |
| 35:BA:1434:A:N3    | 35:BA:1434:A:H2'   | 2.34                     | 0.43              |
| 35:BA:1349:A:N6    | 35:BA:1598:C:N4    | 2.67                     | 0.43              |
| 35:BA:1843:C:H2'   | 35:BA:1844:C:H6    | 1.84                     | 0.43              |
| 35:BA:1930:G:O2'   | 35:BA:1931:U:O5'   | 2.36                     | 0.43              |
| 35:BA:2116:G:N7    | 35:BA:2117:A:C4    | 2.87                     | 0.43              |
| 35:BA:2167:U:H2'   | 35:BA:2168:G:O4'   | 2.18                     | 0.43              |
| 35:BA:2483:C:H5'   | 35:BA:2484:G:OP2   | 2.19                     | 0.43              |
| 35:BA:2876:G:OP1   | 52:BT:2:ASN:O      | 2.37                     | 0.43              |
| 35:BA:329:G:H4'    | 35:BA:330:A:OP2    | 2.17                     | 0.43              |
| 35:BA:331:A:O2'    | 35:BA:332:A:OP1    | 2.27                     | 0.43              |
| 35:BA:525:U:O2'    | 35:BA:526:A:H5''   | 2.19                     | 0.43              |
| 35:BA:797:C:H2'    | 35:BA:798:G:C8     | 2.53                     | 0.43              |
| 35:BA:950:G:H2'    | 35:BA:951:C:C6     | 2.53                     | 0.43              |
| 36:BB:25:A:C2      | 36:BB:26:A:C4      | 3.07                     | 0.43              |
| 36:BB:51:G:H5'     | 36:BB:52:A:OP2     | 2.18                     | 0.43              |
| 36:BB:5:C:O2'      | 36:BB:6:C:H5'      | 2.19                     | 0.43              |
| 37:BC:139:PRO:HA   | 37:BC:145:THR:CB   | 2.49                     | 0.43              |
| 39:BE:161:GLY:O    | 39:BE:162:ALA:C    | 2.57                     | 0.43              |
| 39:BE:165:VAL:HB   | 39:BE:189:PRO:HB3  | 2.01                     | 0.43              |
| 40:BF:160:ASN:HD22 | 40:BF:160:ASN:C    | 2.21                     | 0.43              |
| 40:BF:7:TYR:CD2    | 40:BF:16:GLY:CA    | 2.99                     | 0.43              |
| 40:BF:170:LEU:N    | 40:BF:170:LEU:CD2  | 2.81                     | 0.43              |
| 41:BG:97:ASP:O     | 41:BG:101:ILE:HG13 | 2.18                     | 0.43              |
| 41:BG:108:ASN:O    | 41:BG:109:VAL:CG2  | 2.62                     | 0.43              |
| 41:BG:129:GLY:O    | 41:BG:130:ASN:CG   | 2.56                     | 0.43              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 42:BH:52:VAL:O    | 42:BH:52:VAL:HG12 | 2.18                     | 0.43              |
| 44:BK:3:LYS:HE3   | 44:BK:3:LYS:HB3   | 1.78                     | 0.43              |
| 46:BN:99:LEU:O    | 46:BN:102:ALA:HB3 | 2.18                     | 0.43              |
| 46:BN:2:LYS:HZ3   | 54:BV:12:TYR:HA   | 1.82                     | 0.43              |
| 48:BP:113:LYS:HA  | 48:BP:129:ALA:O   | 2.19                     | 0.43              |
| 48:BP:64:LYS:O    | 48:BP:66:GLY:N    | 2.42                     | 0.43              |
| 51:BS:68:GLN:C    | 51:BS:70:GLY:N    | 2.72                     | 0.43              |
| 36:BB:48:A:OP1    | 51:BS:93:LYS:HB3  | 2.18                     | 0.43              |
| 52:BT:10:VAL:C    | 52:BT:12:SER:H    | 2.22                     | 0.43              |
| 55:BW:47:VAL:HG12 | 55:BW:47:VAL:O    | 2.18                     | 0.43              |
| 58:BZ:120:ILE:HB  | 58:BZ:172:ALA:HA  | 2.01                     | 0.43              |
| 58:BZ:54:HIS:HA   | 58:BZ:98:MET:HE1  | 2.01                     | 0.43              |
| 1:CA:1298:C:C5    | 7:CG:114:ARG:HD3  | 2.53                     | 0.43              |
| 1:CA:1499:A:O2'   | 1:CA:1500:A:H5'   | 2.19                     | 0.43              |
| 1:CA:732:C:H2'    | 1:CA:733:A:H5''   | 2.01                     | 0.43              |
| 2:CB:137:ARG:NH1  | 2:CB:137:ARG:HG2  | 2.34                     | 0.43              |
| 2:CB:142:LEU:HD23 | 2:CB:142:LEU:C    | 2.38                     | 0.43              |
| 3:CC:111:LEU:CD2  | 3:CC:141:VAL:HG13 | 2.49                     | 0.43              |
| 4:CD:9:CYS:SG     | 4:CD:22:LYS:HD2   | 2.58                     | 0.43              |
| 9:CI:11:LYS:O     | 9:CI:11:LYS:HG2   | 2.18                     | 0.43              |
| 9:CI:73:GLN:O     | 9:CI:75:ASP:N     | 2.52                     | 0.43              |
| 13:CM:91:ARG:HD3  | 13:CM:97:PRO:O    | 2.19                     | 0.43              |
| 15:CO:26:GLU:OE2  | 15:CO:77:ARG:HB2  | 2.18                     | 0.43              |
| 19:CS:61:TYR:CG   | 19:CS:62:ILE:N    | 2.87                     | 0.43              |
| 20:CT:58:LYS:O    | 20:CT:59:ALA:C    | 2.57                     | 0.43              |
| 24:CY:302:HIS:C   | 24:CY:304:ASP:H   | 2.22                     | 0.43              |
| 24:CY:651:GLU:OE1 | 24:CY:651:GLU:HA  | 2.18                     | 0.43              |
| 27:D2:50:ILE:HG23 | 27:D2:54:LYS:HE3  | 2.00                     | 0.43              |
| 28:D3:6:VAL:O     | 28:D3:6:VAL:HG23  | 2.19                     | 0.43              |
| 29:D4:26:SER:OG   | 29:D4:27:THR:N    | 2.51                     | 0.43              |
| 35:DA:1385:G:H1'  | 35:DA:1386:C:C6   | 2.53                     | 0.43              |
| 35:DA:2154:G:H2'  | 35:DA:2155:G:C8   | 2.54                     | 0.43              |
| 35:DA:2219:G:H8   | 35:DA:2219:G:O5'  | 2.01                     | 0.43              |
| 35:DA:2080:G:C2   | 35:DA:2241:A:C2   | 3.07                     | 0.43              |
| 35:DA:2552:U:C2   | 35:DA:2554:U:C5'  | 3.01                     | 0.43              |
| 35:DA:512:G:O2'   | 35:DA:513:A:H8    | 2.02                     | 0.43              |
| 36:DB:90:A:C8     | 36:DB:91:C:H1'    | 2.54                     | 0.43              |
| 38:DD:144:ALA:HB3 | 38:DD:192:THR:CG2 | 2.44                     | 0.43              |
| 38:DD:213:ARG:O   | 38:DD:215:LEU:N   | 2.52                     | 0.43              |
| 38:DD:43:ARG:NH1  | 38:DD:49:ILE:HG22 | 2.32                     | 0.43              |
| 39:DE:45:THR:O    | 39:DE:46:ALA:CB   | 2.66                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:DF:132:VAL:O   | 40:DF:133:ASN:HB2  | 2.19                     | 0.43              |
| 46:DN:99:LEU:O    | 46:DN:102:ALA:HB3  | 2.19                     | 0.43              |
| 46:DN:34:LEU:O    | 46:DN:116:LEU:HD22 | 2.18                     | 0.43              |
| 46:DN:22:THR:HB   | 46:DN:25:ARG:CB    | 2.46                     | 0.43              |
| 46:DN:43:THR:HG22 | 46:DN:45:ASN:HD22  | 1.84                     | 0.43              |
| 47:DO:60:ALA:HA   | 47:DO:87:ILE:HD11  | 2.01                     | 0.43              |
| 30:D5:44:THR:CG2  | 50:DR:101:ALA:HB2  | 2.30                     | 0.43              |
| 50:DR:106:GLY:O   | 50:DR:107:ASP:HB3  | 2.17                     | 0.43              |
| 55:DW:44:ALA:O    | 55:DW:45:TYR:C     | 2.57                     | 0.43              |
| 56:DX:41:ASN:HA   | 56:DX:44:GLU:HG2   | 2.00                     | 0.43              |
| 1:AA:1171:G:H2'   | 1:AA:1172:C:C6     | 2.53                     | 0.43              |
| 1:AA:1202:G:H2'   | 1:AA:1203:C:H5'    | 2.00                     | 0.43              |
| 1:AA:1347:G:H2'   | 1:AA:1373:G:N1     | 2.34                     | 0.43              |
| 1:AA:417:C:H2'    | 1:AA:418:C:H6      | 1.84                     | 0.43              |
| 1:AA:509:A:H5'    | 1:AA:510:A:P       | 2.51                     | 0.43              |
| 1:AA:666:G:N2     | 1:AA:667:G:H1'     | 2.34                     | 0.43              |
| 1:AA:714:G:H2'    | 1:AA:715:A:C8      | 2.53                     | 0.43              |
| 1:AA:786:G:C2     | 1:AA:787:A:C4      | 3.07                     | 0.43              |
| 2:AB:117:GLU:O    | 2:AB:120:ALA:HB3   | 2.19                     | 0.43              |
| 3:AC:113:ALA:HB3  | 3:AC:114:PRO:HD3   | 2.00                     | 0.43              |
| 4:AD:92:VAL:O     | 4:AD:95:GLY:N      | 2.52                     | 0.43              |
| 5:AE:69:VAL:HA    | 5:AE:70:PRO:HD2    | 1.82                     | 0.43              |
| 7:AG:79:ARG:O     | 7:AG:79:ARG:HD2    | 2.19                     | 0.43              |
| 10:AJ:4:ILE:CD1   | 10:AJ:4:ILE:N      | 2.79                     | 0.43              |
| 9:AI:114:TYR:CD1  | 10:AJ:60:ARG:HG3   | 2.53                     | 0.43              |
| 12:AL:37:CYS:HB3  | 12:AL:79:GLU:O     | 2.18                     | 0.43              |
| 12:AL:86:ARG:NH2  | 12:AL:99:HIS:CG    | 2.87                     | 0.43              |
| 15:AO:26:GLU:OE2  | 15:AO:77:ARG:HB2   | 2.19                     | 0.43              |
| 19:AS:57:HIS:O    | 19:AS:59:PRO:HD3   | 2.19                     | 0.43              |
| 19:AS:65:ASN:HA   | 29:B4:48:ARG:CZ    | 2.49                     | 0.43              |
| 24:AY:138:LYS:HG2 | 62:AY:703:GDP:C6   | 2.54                     | 0.43              |
| 24:AY:315:LYS:HZ2 | 24:AY:317:MET:HG2  | 1.83                     | 0.43              |
| 24:AY:350:GLU:HG3 | 24:AY:380:LEU:HG   | 2.01                     | 0.43              |
| 24:AY:641:GLN:HB2 | 24:AY:641:GLN:HE21 | 1.63                     | 0.43              |
| 24:AY:5:VAL:C     | 24:AY:7:TYR:H      | 2.22                     | 0.43              |
| 26:B1:44:PRO:C    | 26:B1:46:LEU:HD13  | 2.39                     | 0.43              |
| 27:B2:59:ARG:O    | 27:B2:60:LEU:C     | 2.57                     | 0.43              |
| 31:B6:17:LYS:CB   | 31:B6:44:ARG:NH1   | 2.82                     | 0.43              |
| 32:B7:8:ASN:HD22  | 32:B7:8:ASN:C      | 2.18                     | 0.43              |
| 33:B8:9:GLY:O     | 33:B8:13:ARG:HG2   | 2.19                     | 0.43              |
| 35:BA:1114:G:O2'  | 35:BA:1115:G:H5''  | 2.19                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:BA:1149:G:H2'  | 35:BA:1150:C:H6    | 1.83                     | 0.43              |
| 35:BA:1263:U:C4   | 35:BA:1264:G:C6    | 3.06                     | 0.43              |
| 35:BA:1680:U:O2   | 35:BA:1763:G:H3'   | 2.18                     | 0.43              |
| 35:BA:1947:C:H2'  | 35:BA:1948:G:H8    | 1.82                     | 0.43              |
| 35:BA:2219:G:C2'  | 35:BA:2220:G:H5'   | 2.49                     | 0.43              |
| 35:BA:2345:G:N7   | 35:BA:2372:G:C2    | 2.87                     | 0.43              |
| 35:BA:945:A:C2    | 35:BA:2448:A:N1    | 2.87                     | 0.43              |
| 35:BA:2881:C:C2   | 35:BA:2882:A:C8    | 3.06                     | 0.43              |
| 35:BA:36:G:H4'    | 35:BA:451:C:C2     | 2.54                     | 0.43              |
| 35:BA:420:C:H2'   | 35:BA:421:U:C6     | 2.54                     | 0.43              |
| 35:BA:78:A:H2'    | 35:BA:79:G:H8      | 1.84                     | 0.43              |
| 35:BA:87:C:OP2    | 35:BA:90:U:O4      | 2.37                     | 0.43              |
| 37:BC:127:LYS:O   | 37:BC:128:LEU:HD23 | 2.18                     | 0.43              |
| 37:BC:148:PHE:C   | 37:BC:150:ILE:H    | 2.21                     | 0.43              |
| 35:BA:2785:C:H1'  | 39:BE:64:LYS:NZ    | 2.34                     | 0.43              |
| 40:BF:117:ARG:NH1 | 40:BF:120:GLU:OE1  | 2.52                     | 0.43              |
| 40:BF:133:ASN:O   | 40:BF:134:GLY:C    | 2.57                     | 0.43              |
| 40:BF:198:ALA:HA  | 40:BF:201:VAL:HG12 | 2.01                     | 0.43              |
| 41:BG:56:ALA:HB2  | 41:BG:153:ARG:NH2  | 2.34                     | 0.43              |
| 41:BG:59:GLU:C    | 41:BG:61:ALA:H     | 2.22                     | 0.43              |
| 41:BG:9:ARG:HG2   | 41:BG:13:GLU:OE1   | 2.18                     | 0.43              |
| 44:BK:75:SER:C    | 44:BK:78:ILE:HG22  | 2.38                     | 0.43              |
| 44:BK:8:VAL:CG1   | 44:BK:10:LEU:HG    | 2.47                     | 0.43              |
| 47:BO:104:ARG:CZ  | 52:BT:33:LYS:HD2   | 2.48                     | 0.43              |
| 49:BQ:21:THR:OG1  | 49:BQ:99:PRO:O     | 2.37                     | 0.43              |
| 51:BS:104:GLY:O   | 51:BS:106:ARG:N    | 2.47                     | 0.43              |
| 51:BS:25:ARG:CG   | 51:BS:26:LEU:H     | 2.30                     | 0.43              |
| 51:BS:77:ALA:HB1  | 51:BS:82:ILE:HB    | 2.00                     | 0.43              |
| 53:BU:29:SER:OG   | 53:BU:30:LYS:HE2   | 2.19                     | 0.43              |
| 55:BW:70:TYR:HB3  | 55:BW:110:LYS:NZ   | 2.33                     | 0.43              |
| 55:BW:72:LYS:H    | 55:BW:107:LEU:HA   | 1.84                     | 0.43              |
| 1:CA:1002:G:C8    | 1:CA:1003:G:N7     | 2.86                     | 0.43              |
| 1:CA:1008:C:O5'   | 1:CA:1008:C:H6     | 2.02                     | 0.43              |
| 1:CA:1065:U:O2'   | 1:CA:1066:C:OP2    | 2.37                     | 0.43              |
| 1:CA:1218:C:H2'   | 1:CA:1219:U:C5     | 2.54                     | 0.43              |
| 1:CA:1260:C:O5'   | 1:CA:1284:C:H4'    | 2.18                     | 0.43              |
| 1:CA:1360:A:H2'   | 1:CA:1361:G:C8     | 2.53                     | 0.43              |
| 1:CA:143:A:N1     | 1:CA:220:G:O6      | 2.52                     | 0.43              |
| 1:CA:40:C:H2'     | 1:CA:41:G:H8       | 1.82                     | 0.43              |
| 1:CA:786:G:C2     | 1:CA:787:A:C4      | 3.06                     | 0.43              |
| 2:CB:207:ALA:C    | 2:CB:209:ARG:N     | 2.70                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 2:CB:213:LEU:C      | 2:CB:213:LEU:HD23 | 2.39                     | 0.43              |
| 3:CC:140:ARG:NH1    | 3:CC:140:ARG:HG3  | 2.34                     | 0.43              |
| 3:CC:43:LEU:C       | 3:CC:45:LYS:H     | 2.22                     | 0.43              |
| 3:CC:50:ALA:HA      | 3:CC:72:LYS:HB3   | 2.01                     | 0.43              |
| 4:CD:121:VAL:CA     | 4:CD:126:ILE:HD13 | 2.47                     | 0.43              |
| 4:CD:132:ARG:C      | 4:CD:132:ARG:HD2  | 2.38                     | 0.43              |
| 5:CE:143:ARG:HH12   | 8:CH:77:GLU:CD    | 2.22                     | 0.43              |
| 5:CE:147:ASP:HA     | 5:CE:150:ARG:NH1  | 2.34                     | 0.43              |
| 5:CE:78:HIS:HE1     | 5:CE:80:ILE:CG2   | 2.30                     | 0.43              |
| 7:CG:113:GLU:CG     | 7:CG:119:ARG:HG2  | 2.48                     | 0.43              |
| 8:CH:122:ARG:HB3    | 8:CH:122:ARG:HH11 | 1.83                     | 0.43              |
| 8:CH:66:GLY:O       | 8:CH:76:PRO:HB3   | 2.18                     | 0.43              |
| 12:CL:44:THR:HA     | 12:CL:45:PRO:HD3  | 1.79                     | 0.43              |
| 13:CM:66:LEU:O      | 13:CM:67:GLU:O    | 2.37                     | 0.43              |
| 14:CN:24:CYS:SG     | 14:CN:39:LEU:HA   | 2.59                     | 0.43              |
| 15:CO:18:PHE:O      | 15:CO:18:PHE:CD1  | 2.71                     | 0.43              |
| 18:CR:79:LEU:HD23   | 18:CR:79:LEU:HA   | 1.91                     | 0.43              |
| 13:CM:94:ARG:CZ     | 19:CS:82:GLY:N    | 2.81                     | 0.43              |
| 1:CA:1352:C:OP1     | 21:CU:3:LYS:CE    | 2.67                     | 0.43              |
| 22:CW:66:C:C4       | 22:CW:67:C:N4     | 2.86                     | 0.43              |
| 24:CY:261:GLY:O     | 24:CY:262:SER:C   | 2.56                     | 0.43              |
| 26:D1:34:THR:HG21   | 26:D1:37:ILE:HG13 | 2.01                     | 0.43              |
| 26:D1:4:VAL:CG2     | 26:D1:5:CYS:N     | 2.81                     | 0.43              |
| 26:D1:75:GLU:OE1    | 26:D1:75:GLU:HA   | 2.18                     | 0.43              |
| 33:D8:61:LEU:N      | 33:D8:63:PRO:HD2  | 2.34                     | 0.43              |
| 33:D8:9:GLY:O       | 33:D8:13:ARG:HG2  | 2.18                     | 0.43              |
| 34:D9:29:ASN:HA     | 34:D9:30:PRO:HD2  | 1.89                     | 0.43              |
| 35:DA:1166:C:H2'    | 35:DA:1167:U:H6   | 1.84                     | 0.43              |
| 35:DA:11:G:H2'      | 35:DA:12:U:H6     | 1.81                     | 0.43              |
| 35:DA:1263:U:H2'    | 35:DA:1264:G:C8   | 2.53                     | 0.43              |
| 35:DA:2291:U:OP1    | 35:DA:2380:C:O2'  | 2.36                     | 0.43              |
| 35:DA:2376:A:H2'    | 35:DA:2377:A:O4'  | 2.18                     | 0.43              |
| 35:DA:2390:U:O2'    | 35:DA:2391:G:H5'  | 2.18                     | 0.43              |
| 35:DA:2801(A):A:H4' | 35:DA:2802:G:H8   | 1.81                     | 0.43              |
| 35:DA:2850:A:OP2    | 35:DA:2866:U:H5   | 2.02                     | 0.43              |
| 35:DA:2889:C:H2'    | 35:DA:2891:G:O4'  | 2.19                     | 0.43              |
| 35:DA:299:A:H1'     | 35:DA:322:A:N6    | 2.33                     | 0.43              |
| 35:DA:420:C:H2'     | 35:DA:421:U:C6    | 2.54                     | 0.43              |
| 35:DA:448:U:C4      | 35:DA:583:G:H1'   | 2.54                     | 0.43              |
| 35:DA:483:A:C2      | 35:DA:484:C:C1'   | 3.02                     | 0.43              |
| 35:DA:839:U:H2'     | 35:DA:840:C:H6    | 1.80                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:DB:25:A:C2     | 36:DB:26:A:C4     | 3.06                     | 0.43              |
| 35:DA:2122:U:O2'  | 37:DC:173:HIS:HD2 | 2.01                     | 0.43              |
| 39:DE:152:LYS:HG3 | 39:DE:153:GLY:H   | 1.83                     | 0.43              |
| 35:DA:2785:C:H1'  | 39:DE:64:LYS:NZ   | 2.34                     | 0.43              |
| 40:DF:10:PRO:HB3  | 40:DF:127:GLU:CG  | 2.49                     | 0.43              |
| 40:DF:133:ASN:O   | 40:DF:134:GLY:C   | 2.57                     | 0.43              |
| 40:DF:25:PRO:CB   | 40:DF:119:ARG:HB2 | 2.48                     | 0.43              |
| 42:DH:149:ARG:HA  | 42:DH:162:ILE:CG1 | 2.48                     | 0.43              |
| 46:DN:109:LYS:HE3 | 46:DN:109:LYS:H   | 1.84                     | 0.43              |
| 46:DN:43:THR:HB   | 46:DN:46:VAL:CG1  | 2.46                     | 0.43              |
| 46:DN:43:THR:HG22 | 46:DN:45:ASN:ND2  | 2.33                     | 0.43              |
| 46:DN:4:TYR:O     | 46:DN:5:VAL:C     | 2.57                     | 0.43              |
| 48:DP:47:ASP:HB3  | 48:DP:48:PRO:C    | 2.39                     | 0.43              |
| 35:DA:2467:C:O2   | 49:DQ:124:LYS:NZ  | 2.52                     | 0.43              |
| 50:DR:101:ALA:O   | 50:DR:102:GLU:HB2 | 2.19                     | 0.43              |
| 50:DR:53:HIS:HD1  | 50:DR:53:HIS:C    | 2.22                     | 0.43              |
| 51:DS:65:VAL:C    | 51:DS:67:ARG:H    | 2.21                     | 0.43              |
| 51:DS:78:LEU:HD11 | 51:DS:103:GLU:HB3 | 2.01                     | 0.43              |
| 39:DE:15:PHE:CZ   | 52:DT:80:SER:HB2  | 2.54                     | 0.43              |
| 53:DU:112:ARG:CG  | 53:DU:112:ARG:NH1 | 2.82                     | 0.43              |
| 56:DX:57:LEU:HD22 | 56:DX:57:LEU:C    | 2.39                     | 0.43              |
| 35:DA:64:A:C5     | 56:DX:66:LEU:HD13 | 2.54                     | 0.43              |
| 36:DB:76:G:H21    | 58:DZ:75:ASN:HD22 | 1.66                     | 0.43              |
| 1:AA:1037:C:H2'   | 1:AA:1038:C:N1    | 2.33                     | 0.43              |
| 1:AA:1209:C:O2'   | 1:AA:1210:C:H5'   | 2.18                     | 0.43              |
| 1:AA:1237:C:H3'   | 1:AA:1336:C:N4    | 2.33                     | 0.43              |
| 1:AA:976:G:H5'    | 1:AA:1358:U:O2'   | 2.18                     | 0.43              |
| 1:AA:1360:A:H2'   | 1:AA:1361:G:C8    | 2.53                     | 0.43              |
| 1:AA:1411:C:O2    | 1:AA:1411:C:H2'   | 2.19                     | 0.43              |
| 1:AA:1522:U:H2'   | 1:AA:1523:G:C8    | 2.49                     | 0.43              |
| 1:AA:277:C:C2'    | 1:AA:278:G:H5'    | 2.49                     | 0.43              |
| 1:AA:342:C:C5     | 1:AA:343:U:C5     | 3.06                     | 0.43              |
| 1:AA:47:C:H6      | 1:AA:365:U:H2'    | 1.84                     | 0.43              |
| 1:AA:450:G:H1     | 1:AA:483:C:H42    | 1.66                     | 0.43              |
| 1:AA:66:G:C4'     | 1:AA:173:U:C5     | 3.00                     | 0.43              |
| 1:AA:954:G:H2'    | 1:AA:955:U:O4'    | 2.18                     | 0.43              |
| 1:AA:965:A:C2     | 1:AA:969:A:N1     | 2.87                     | 0.43              |
| 2:AB:39:ILE:HG22  | 2:AB:41:ILE:HD12  | 2.00                     | 0.43              |
| 4:AD:96:LEU:O     | 4:AD:99:SER:N     | 2.51                     | 0.43              |
| 5:AE:139:LEU:C    | 5:AE:141:GLN:N    | 2.72                     | 0.43              |
| 7:AG:85:TYR:CD1   | 7:AG:154:TYR:HE1  | 2.37                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:AH:44:PHE:HE2    | 8:AH:109:ILE:HG21  | 1.83                     | 0.43              |
| 8:AH:6:ILE:O       | 8:AH:9:MET:N       | 2.52                     | 0.43              |
| 10:AJ:98:ILE:CG2   | 10:AJ:98:ILE:O     | 2.66                     | 0.43              |
| 13:AM:66:LEU:HA    | 13:AM:70:LEU:HD13  | 2.01                     | 0.43              |
| 18:AR:66:LEU:HG    | 18:AR:70:ILE:CD1   | 2.49                     | 0.43              |
| 18:AR:72:ARG:O     | 18:AR:73:ALA:C     | 2.57                     | 0.43              |
| 11:AK:109:VAL:HG13 | 18:AR:85:LEU:O     | 2.19                     | 0.43              |
| 20:AT:22:ARG:O     | 20:AT:26:ASN:ND2   | 2.52                     | 0.43              |
| 24:AY:208:GLN:O    | 24:AY:209:ALA:O    | 2.37                     | 0.43              |
| 24:AY:238:THR:HG23 | 24:AY:240:GLU:HG2  | 2.00                     | 0.43              |
| 24:AY:282:SER:C    | 24:AY:284:LEU:N    | 2.72                     | 0.43              |
| 24:AY:415:PRO:HB2  | 24:AY:421:GLN:HA   | 2.00                     | 0.43              |
| 24:AY:447:GLY:O    | 24:AY:448:GLN:O    | 2.36                     | 0.43              |
| 24:AY:539:ILE:N    | 24:AY:540:PRO:CD   | 2.81                     | 0.43              |
| 24:AY:609:GLU:HB2  | 24:AY:670:VAL:CG2  | 2.49                     | 0.43              |
| 29:B4:31:ILE:O     | 29:B4:31:ILE:HG22  | 2.18                     | 0.43              |
| 35:BA:1174:A:H5'   | 35:BA:1175:U:H5''  | 2.01                     | 0.43              |
| 35:BA:1463:C:H2'   | 35:BA:1464:C:H6    | 1.82                     | 0.43              |
| 35:BA:1567:A:OP2   | 38:BD:84:TYR:OH    | 2.33                     | 0.43              |
| 35:BA:1570:A:H2'   | 35:BA:1571:A:C8    | 2.54                     | 0.43              |
| 35:BA:1765:C:H2'   | 35:BA:1766:U:H6    | 1.83                     | 0.43              |
| 35:BA:2197:U:H1'   | 35:BA:2198:A:C8    | 2.53                     | 0.43              |
| 35:BA:2578:G:N2    | 35:BA:2579:C:C2    | 2.87                     | 0.43              |
| 35:BA:271(E):U:H3  | 35:BA:271(S):G:H1  | 1.66                     | 0.43              |
| 35:BA:2848:G:OP2   | 52:BT:97:ALA:N     | 2.49                     | 0.43              |
| 35:BA:2849:U:H1'   | 35:BA:2866:U:H6    | 1.84                     | 0.43              |
| 35:BA:361:G:N2     | 35:BA:362:U:H1'    | 2.34                     | 0.43              |
| 35:BA:565:C:O2'    | 35:BA:566:U:H5'    | 2.19                     | 0.43              |
| 35:BA:581:C:C2     | 35:BA:582:G:N7     | 2.87                     | 0.43              |
| 36:BB:89:G:C6      | 36:BB:90:A:N1      | 2.87                     | 0.43              |
| 36:BB:96:U:H2'     | 36:BB:97:G:H8      | 1.84                     | 0.43              |
| 37:BC:135:ARG:C    | 37:BC:137:LEU:H    | 2.22                     | 0.43              |
| 37:BC:149:ASN:ND2  | 37:BC:149:ASN:C    | 2.72                     | 0.43              |
| 35:BA:2821:A:OP2   | 39:BE:110:GLY:O    | 2.37                     | 0.43              |
| 35:BA:2531:A:H4'   | 42:BH:157:TYR:CD2  | 2.53                     | 0.43              |
| 42:BH:92:ILE:HG22  | 42:BH:93:GLY:N     | 2.33                     | 0.43              |
| 44:BK:4:VAL:CG1    | 44:BK:5:VAL:H      | 2.10                     | 0.43              |
| 47:BO:120:GLU:OE2  | 47:BO:122:LEU:HD21 | 2.18                     | 0.43              |
| 47:BO:24:VAL:CG2   | 47:BO:24:VAL:O     | 2.66                     | 0.43              |
| 48:BP:98:GLU:O     | 48:BP:102:ARG:NH2  | 2.52                     | 0.43              |
| 51:BS:13:ARG:CG    | 51:BS:14:VAL:N     | 2.64                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:BS:63:THR:O     | 51:BS:66:ALA:N     | 2.51                     | 0.43              |
| 55:BW:12:ILE:CG1   | 55:BW:42:ARG:NH1   | 2.81                     | 0.43              |
| 57:BY:54:LYS:HE2   | 57:BY:55:TYR:HE2   | 1.84                     | 0.43              |
| 58:BZ:81:ARG:NH1   | 58:BZ:81:ARG:HB3   | 2.34                     | 0.43              |
| 1:CA:1347:G:H2'    | 1:CA:1373:G:N1     | 2.34                     | 0.43              |
| 1:CA:398:C:H2'     | 1:CA:399:G:H8      | 1.84                     | 0.43              |
| 1:CA:499:A:O2'     | 1:CA:500:G:C8      | 2.65                     | 0.43              |
| 1:CA:596:C:OP2     | 1:CA:597:G:OP2     | 2.37                     | 0.43              |
| 1:CA:61:G:H2'      | 1:CA:62:U:O4'      | 2.19                     | 0.43              |
| 1:CA:785:G:C2'     | 1:CA:786:G:H5'     | 2.48                     | 0.43              |
| 1:CA:822:C:O2'     | 1:CA:823:G:H5'     | 2.18                     | 0.43              |
| 2:CB:142:LEU:CD2   | 2:CB:146:GLN:NE2   | 2.82                     | 0.43              |
| 2:CB:178:ARG:CB    | 2:CB:178:ARG:HH11  | 2.31                     | 0.43              |
| 2:CB:233:SER:HB2   | 2:CB:234:PRO:HD3   | 1.98                     | 0.43              |
| 2:CB:95:GLN:HA     | 2:CB:95:GLN:OE1    | 2.19                     | 0.43              |
| 3:CC:131:ARG:O     | 3:CC:132:ARG:C     | 2.56                     | 0.43              |
| 3:CC:70:VAL:HG21   | 3:CC:76:VAL:HG11   | 2.00                     | 0.43              |
| 4:CD:108:LEU:HD23  | 4:CD:110:PHE:CZ    | 2.53                     | 0.43              |
| 4:CD:129:ASN:N     | 4:CD:129:ASN:ND2   | 2.66                     | 0.43              |
| 1:CA:405:U:OP2     | 4:CD:3:ARG:HD2     | 2.19                     | 0.43              |
| 5:CE:78:HIS:ND1    | 5:CE:79:GLU:N      | 2.67                     | 0.43              |
| 7:CG:65:ALA:HB2    | 7:CG:128:ALA:HB2   | 2.00                     | 0.43              |
| 9:CI:42:ARG:O      | 9:CI:43:ALA:C      | 2.57                     | 0.43              |
| 13:CM:106:ASN:O    | 13:CM:107:ALA:CB   | 2.67                     | 0.43              |
| 13:CM:29:ARG:HB3   | 13:CM:64:TRP:CZ2   | 2.54                     | 0.43              |
| 13:CM:91:ARG:CD    | 13:CM:97:PRO:O     | 2.67                     | 0.43              |
| 15:CO:82:ILE:CD1   | 15:CO:82:ILE:C     | 2.82                     | 0.43              |
| 24:CY:226:ASN:O    | 24:CY:228:MET:N    | 2.51                     | 0.43              |
| 24:CY:315:LYS:NZ   | 24:CY:317:MET:CG   | 2.82                     | 0.43              |
| 24:CY:495:GLY:O    | 24:CY:509:HIS:HA   | 2.18                     | 0.43              |
| 24:CY:621:ILE:HD12 | 35:DA:1095:A:H1'   | 2.01                     | 0.43              |
| 30:D5:16:ARG:HG2   | 30:D5:16:ARG:HH11  | 1.84                     | 0.43              |
| 31:D6:51:GLU:HG2   | 31:D6:52:VAL:N     | 2.31                     | 0.43              |
| 35:DA:83:G:N2      | 35:DA:103:A:OP2    | 2.52                     | 0.43              |
| 35:DA:1315:C:H42   | 35:DA:1337:G:H1    | 1.66                     | 0.43              |
| 35:DA:1654:A:O2'   | 39:DE:113:PHE:O    | 2.37                     | 0.43              |
| 35:DA:2089:U:O2'   | 35:DA:2090:G:H5'   | 2.18                     | 0.43              |
| 35:DA:332:A:H4'    | 35:DA:333:G:OP1    | 2.19                     | 0.43              |
| 35:DA:930:U:H4'    | 35:DA:931:G:O5'    | 2.19                     | 0.43              |
| 37:DC:139:PRO:HA   | 37:DC:145:THR:HG21 | 2.01                     | 0.43              |
| 37:DC:29:LEU:CD2   | 37:DC:29:LEU:C     | 2.88                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:DA:1971:A:N3    | 38:DD:241:PRO:HD3 | 2.34                     | 0.43              |
| 35:DA:1814:G:C4'   | 38:DD:51:VAL:HG21 | 2.49                     | 0.43              |
| 35:DA:2572:A:C8    | 39:DE:144:ARG:CB  | 3.02                     | 0.43              |
| 39:DE:31:CYS:HB3   | 39:DE:49:LEU:HB3  | 2.00                     | 0.43              |
| 39:DE:9:VAL:HG22   | 39:DE:25:VAL:HB   | 2.01                     | 0.43              |
| 41:DG:97:ASP:O     | 41:DG:101:ILE:HB  | 2.18                     | 0.43              |
| 42:DH:38:SER:HA    | 42:DH:39:PRO:HD3  | 1.84                     | 0.43              |
| 49:DQ:132:VAL:HB   | 49:DQ:137:TYR:OH  | 2.19                     | 0.43              |
| 49:DQ:69:PHE:CD1   | 49:DQ:70:PRO:HD2  | 2.53                     | 0.43              |
| 52:DT:14:TYR:CD1   | 52:DT:14:TYR:N    | 2.87                     | 0.43              |
| 54:DV:38:LEU:C     | 54:DV:39:LEU:HD22 | 2.39                     | 0.43              |
| 58:DZ:133:ILE:N    | 58:DZ:134:PRO:CD  | 2.81                     | 0.43              |
| 58:DZ:25:PRO:HA    | 58:DZ:38:TYR:CB   | 2.49                     | 0.43              |
| 1:AA:534:U:H5'     | 1:AA:534:U:H6     | 1.84                     | 0.43              |
| 1:AA:596:C:H6      | 1:AA:596:C:O5'    | 2.02                     | 0.43              |
| 1:AA:769:G:O2'     | 1:AA:770:C:H5'    | 2.19                     | 0.43              |
| 5:AE:78:HIS:HE1    | 5:AE:80:ILE:HG23  | 1.83                     | 0.43              |
| 9:AI:46:ALA:C      | 9:AI:47:LEU:HD12  | 2.39                     | 0.43              |
| 9:AI:56:LEU:HD23   | 9:AI:56:LEU:O     | 2.19                     | 0.43              |
| 13:AM:10:PRO:O     | 13:AM:11:ARG:CB   | 2.66                     | 0.43              |
| 15:AO:33:THR:HG23  | 15:AO:63:ARG:NH1  | 2.33                     | 0.43              |
| 1:AA:322:C:H4'     | 20:AT:23:ARG:HD2  | 2.01                     | 0.43              |
| 21:AU:8:THR:O      | 21:AU:9:ARG:C     | 2.56                     | 0.43              |
| 22:AV:9:G:N3       | 22:AV:45:G:H2'    | 2.33                     | 0.43              |
| 24:AY:166:LEU:HD21 | 24:AY:212:TYR:CD2 | 2.53                     | 0.43              |
| 24:AY:229:LEU:O    | 24:AY:231:TYR:N   | 2.52                     | 0.43              |
| 24:AY:276:VAL:HG12 | 24:AY:277:VAL:N   | 2.34                     | 0.43              |
| 24:AY:415:PRO:HB2  | 24:AY:421:GLN:N   | 2.34                     | 0.43              |
| 24:AY:623:ASP:HB2  | 24:AY:662:LYS:HE3 | 2.01                     | 0.43              |
| 24:AY:659:LEU:HD13 | 24:AY:659:LEU:O   | 2.18                     | 0.43              |
| 27:B2:36:ARG:O     | 27:B2:37:PHE:C    | 2.56                     | 0.43              |
| 28:B3:1:MET:HB3    | 28:B3:2:PRO:HD2   | 2.01                     | 0.43              |
| 29:B4:28:LYS:HE3   | 29:B4:28:LYS:HA   | 2.01                     | 0.43              |
| 30:B5:48:GLU:C     | 30:B5:49:CYS:SG   | 2.98                     | 0.43              |
| 31:B6:17:LYS:O     | 31:B6:18:ARG:O    | 2.37                     | 0.43              |
| 35:BA:1161:C:H2'   | 35:BA:1162:G:C8   | 2.54                     | 0.43              |
| 35:BA:143(A):C:H2' | 35:BA:143(A):C:O2 | 2.17                     | 0.43              |
| 35:BA:1545:A:N7    | 35:BA:1546:C:C2   | 2.86                     | 0.43              |
| 35:BA:186:G:C2     | 35:BA:211:A:C2    | 3.06                     | 0.43              |
| 35:BA:2488:A:H2'   | 35:BA:2489:G:C8   | 2.54                     | 0.43              |
| 35:BA:2576:G:H3'   | 35:BA:2576:G:N3   | 2.33                     | 0.43              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:BA:2615:U:H2'  | 35:BA:2616:C:H6    | 1.84                     | 0.43              |
| 35:BA:272(I):U:C5 | 35:BA:363(A):A:C2  | 3.07                     | 0.43              |
| 35:BA:545:C:C3'   | 35:BA:547:A:C5'    | 2.95                     | 0.43              |
| 35:BA:708:C:H42   | 35:BA:723:G:H1     | 1.67                     | 0.43              |
| 35:BA:739:G:OP2   | 35:BA:739:G:H8     | 2.02                     | 0.43              |
| 35:BA:769:G:HO2'  | 35:BA:770:G:H5'    | 1.81                     | 0.43              |
| 35:BA:833:U:OP1   | 48:BP:45:LEU:HD21  | 2.18                     | 0.43              |
| 35:BA:977:G:H2'   | 35:BA:978:G:H8     | 1.83                     | 0.43              |
| 39:BE:68:ALA:C    | 39:BE:70:ALA:H     | 2.22                     | 0.43              |
| 39:BE:51:PHE:O    | 39:BE:74:PRO:HB3   | 2.18                     | 0.43              |
| 40:BF:10:PRO:HB3  | 40:BF:127:GLU:CG   | 2.49                     | 0.43              |
| 40:BF:17:ARG:HG3  | 40:BF:17:ARG:NH1   | 2.34                     | 0.43              |
| 41:BG:162:THR:O   | 41:BG:163:ALA:C    | 2.56                     | 0.43              |
| 41:BG:34:LEU:H    | 41:BG:34:LEU:HD12  | 1.83                     | 0.43              |
| 29:B4:1:MET:HE2   | 41:BG:66:GLN:OE1   | 2.18                     | 0.43              |
| 41:BG:39:ILE:HD11 | 41:BG:92:VAL:CG2   | 2.48                     | 0.43              |
| 45:BL:79:UNK:O    | 45:BL:80:UNK:C     | 2.67                     | 0.43              |
| 46:BN:18:ALA:HB1  | 46:BN:21:LYS:HB2   | 2.01                     | 0.43              |
| 46:BN:34:LEU:O    | 46:BN:116:LEU:HD22 | 2.19                     | 0.43              |
| 48:BP:11:GLY:O    | 48:BP:12:ALA:O     | 2.36                     | 0.43              |
| 48:BP:23:PRO:O    | 48:BP:29:LYS:O     | 2.36                     | 0.43              |
| 48:BP:58:THR:O    | 48:BP:61:ARG:HG3   | 2.18                     | 0.43              |
| 54:BV:40:LEU:N    | 54:BV:40:LEU:CD2   | 2.82                     | 0.43              |
| 56:BX:41:ASN:HD22 | 56:BX:41:ASN:N     | 2.16                     | 0.43              |
| 57:BY:13:VAL:HG22 | 57:BY:14:LEU:N     | 2.32                     | 0.43              |
| 57:BY:77:PRO:O    | 57:BY:78:ALA:CB    | 2.67                     | 0.43              |
| 58:BZ:175:VAL:HB  | 58:BZ:176:PRO:HD2  | 2.00                     | 0.43              |
| 1:CA:1003:G:N2    | 1:CA:1004:A:H1'    | 2.33                     | 0.43              |
| 1:CA:1157:A:H4'   | 1:CA:1158:C:O5'    | 2.18                     | 0.43              |
| 1:CA:345:C:H5'    | 1:CA:346:G:OP1     | 2.18                     | 0.43              |
| 1:CA:811:C:H4'    | 1:CA:900:A:N6      | 2.34                     | 0.43              |
| 1:CA:98:G:C2'     | 1:CA:99:U:H5'      | 2.49                     | 0.43              |
| 2:CB:9:GLU:HG2    | 2:CB:10:LEU:N      | 2.34                     | 0.43              |
| 2:CB:58:ILE:H     | 2:CB:58:ILE:HG13   | 1.68                     | 0.43              |
| 3:CC:47:LEU:HB3   | 3:CC:52:LEU:HD22   | 2.00                     | 0.43              |
| 3:CC:77:ILE:O     | 3:CC:84:ILE:HG22   | 2.18                     | 0.43              |
| 4:CD:14:ARG:C     | 4:CD:16:GLY:N      | 2.71                     | 0.43              |
| 5:CE:145:LYS:O    | 5:CE:149:GLU:HG2   | 2.19                     | 0.43              |
| 6:CF:67:MET:CE    | 6:CF:75:LEU:HD22   | 2.49                     | 0.43              |
| 8:CH:100:ILE:HA   | 8:CH:101:PRO:HD3   | 1.74                     | 0.43              |
| 5:CE:155:GLU:N    | 8:CH:64:LYS:HE2    | 2.34                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:CI:20:ARG:O      | 9:CI:60:ASP:N      | 2.44                     | 0.43              |
| 15:CO:27:VAL:O     | 15:CO:31:LEU:HD23  | 2.18                     | 0.43              |
| 15:CO:39:LEU:HD22  | 15:CO:43:LEU:HG    | 2.00                     | 0.43              |
| 16:CP:6:LEU:HD11   | 16:CP:19:ILE:CD1   | 2.49                     | 0.43              |
| 17:CQ:60:ILE:HG22  | 17:CQ:72:ARG:O     | 2.19                     | 0.43              |
| 19:CS:15:LEU:HD13  | 19:CS:31:ILE:HD11  | 2.01                     | 0.43              |
| 20:CT:16:HIS:O     | 20:CT:19:SER:HB3   | 2.18                     | 0.43              |
| 20:CT:22:ARG:O     | 20:CT:26:ASN:ND2   | 2.52                     | 0.43              |
| 20:CT:74:LYS:HB2   | 20:CT:75:ASN:H     | 1.45                     | 0.43              |
| 24:CY:13:ARG:HH11  | 24:CY:277:VAL:HA   | 1.84                     | 0.43              |
| 24:CY:293:THR:HG23 | 24:CY:297:GLU:HG3  | 2.01                     | 0.43              |
| 24:CY:406:GLU:OE1  | 24:CY:406:GLU:N    | 2.31                     | 0.43              |
| 24:CY:428:LEU:N    | 24:CY:428:LEU:HD23 | 2.29                     | 0.43              |
| 24:CY:492:ASP:CG   | 24:CY:512:ILE:O    | 2.58                     | 0.43              |
| 24:CY:84:THR:C     | 61:CY:702:FUA:H322 | 2.39                     | 0.43              |
| 27:D2:13:ALA:O     | 27:D2:14:ARG:C     | 2.56                     | 0.43              |
| 28:D3:22:ALA:HA    | 28:D3:46:ASN:ND2   | 2.33                     | 0.43              |
| 33:D8:56:GLU:C     | 33:D8:58:ILE:H     | 2.23                     | 0.43              |
| 34:D9:1:MET:SD     | 35:DA:2478:A:OP2   | 2.76                     | 0.43              |
| 35:DA:1396:U:O2    | 35:DA:1396:U:C2'   | 2.67                     | 0.43              |
| 35:DA:143:G:H2'    | 35:DA:143(A):C:H6  | 1.84                     | 0.43              |
| 35:DA:1666:G:H2'   | 35:DA:1667:G:H5'   | 2.00                     | 0.43              |
| 35:DA:1836:C:O2'   | 35:DA:1837:C:H5'   | 2.18                     | 0.43              |
| 35:DA:2078:C:H1'   | 35:DA:2434:A:H1'   | 2.01                     | 0.43              |
| 35:DA:406:G:O2'    | 35:DA:407:G:C8     | 2.60                     | 0.43              |
| 35:DA:452:G:N3     | 35:DA:457:A:H2     | 2.16                     | 0.43              |
| 35:DA:527:C:O4'    | 35:DA:527:C:O2     | 2.34                     | 0.43              |
| 35:DA:611:C:H2'    | 35:DA:612:C:H6     | 1.83                     | 0.43              |
| 32:D7:12:ARG:HG3   | 35:DA:686:G:O6     | 2.19                     | 0.43              |
| 35:DA:746:A:HO2'   | 35:DA:2611:U:HO2'  | 1.63                     | 0.43              |
| 35:DA:886:C:H2'    | 35:DA:887:A:O4'    | 2.19                     | 0.43              |
| 35:DA:904:C:C5'    | 35:DA:904:C:H6     | 2.26                     | 0.43              |
| 35:DA:978:G:N2     | 35:DA:979:G:H1'    | 2.34                     | 0.43              |
| 37:DC:184:GLU:OE1  | 37:DC:185:LYS:HD2  | 2.19                     | 0.43              |
| 38:DD:218:ARG:HG3  | 38:DD:218:ARG:NH1  | 2.33                     | 0.43              |
| 38:DD:45:ASN:CG    | 38:DD:46:GLN:H     | 2.21                     | 0.43              |
| 39:DE:26:ILE:HG13  | 39:DE:182:LEU:HB3  | 2.00                     | 0.43              |
| 39:DE:7:VAL:CG1    | 39:DE:27:LEU:HB3   | 2.47                     | 0.43              |
| 40:DF:206:ILE:CG2  | 40:DF:207:GLY:H    | 2.31                     | 0.43              |
| 42:DH:120:GLY:C    | 42:DH:121:ILE:HG13 | 2.38                     | 0.43              |
| 42:DH:137:ASP:HB2  | 42:DH:140:LYS:CD   | 2.47                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 42:DH:149:ARG:HD3  | 42:DH:164:TYR:HE1   | 1.79                     | 0.43              |
| 42:DH:18:GLU:CB    | 42:DH:25:LYS:HB2    | 2.45                     | 0.43              |
| 48:DP:115:LEU:CD2  | 48:DP:115:LEU:N     | 2.81                     | 0.43              |
| 51:DS:40:ILE:HG22  | 51:DS:41:ASP:H      | 1.84                     | 0.43              |
| 52:DT:126:ALA:C    | 52:DT:128:GLU:N     | 2.72                     | 0.43              |
| 52:DT:50:ILE:HD11  | 52:DT:64:ARG:HB3    | 2.00                     | 0.43              |
| 53:DU:53:ARG:HG3   | 53:DU:57:PHE:HE1    | 1.84                     | 0.43              |
| 53:DU:92:ARG:HB3   | 54:DV:11:GLN:NE2    | 2.34                     | 0.43              |
| 55:DW:11:ARG:HD3   | 55:DW:11:ARG:O      | 2.18                     | 0.43              |
| 55:DW:37:ARG:HG3   | 55:DW:38:TYR:CD2    | 2.54                     | 0.43              |
| 55:DW:66:GLU:HA    | 55:DW:69:LEU:HD12   | 2.01                     | 0.43              |
| 58:DZ:125:LEU:HB3  | 58:DZ:165:VAL:HG22  | 2.00                     | 0.43              |
| 58:DZ:17:ALA:C     | 58:DZ:20:ARG:HG2    | 2.38                     | 0.43              |
| 58:DZ:48:PHE:C     | 58:DZ:48:PHE:CD1    | 2.92                     | 0.43              |
| 1:AA:1101:A:H4'    | 1:AA:1102:A:H4'     | 2.01                     | 0.42              |
| 1:AA:1157:A:H4'    | 1:AA:1158:C:O5'     | 2.19                     | 0.42              |
| 1:AA:1442(A):G:O2' | 1:AA:1442(B):A:H5'' | 2.18                     | 0.42              |
| 1:AA:311:C:H2'     | 1:AA:312:C:H6       | 1.84                     | 0.42              |
| 1:AA:318:G:O2'     | 1:AA:319:G:H5'      | 2.19                     | 0.42              |
| 1:AA:360:A:O2'     | 1:AA:361:G:H5'      | 2.19                     | 0.42              |
| 1:AA:556:C:C2'     | 1:AA:557:G:H5'      | 2.50                     | 0.42              |
| 1:AA:674:G:H2'     | 1:AA:675:A:H8       | 1.83                     | 0.42              |
| 2:AB:28:PHE:CE1    | 2:AB:31:TYR:HB2     | 2.54                     | 0.42              |
| 3:AC:101:LEU:HD23  | 3:AC:102:ASN:N      | 2.33                     | 0.42              |
| 3:AC:53:ALA:HB1    | 3:AC:114:PRO:HB2    | 2.01                     | 0.42              |
| 4:AD:170:VAL:O     | 4:AD:171:GLY:C      | 2.57                     | 0.42              |
| 4:AD:30:LYS:HB3    | 4:AD:35:ARG:HD2     | 2.00                     | 0.42              |
| 5:AE:78:HIS:ND1    | 5:AE:79:GLU:N       | 2.67                     | 0.42              |
| 15:AO:17:ARG:NH1   | 15:AO:77:ARG:NH1    | 2.66                     | 0.42              |
| 17:AQ:22:LEU:HD13  | 17:AQ:41:LYS:HG2    | 2.00                     | 0.42              |
| 20:AT:26:ASN:HD22  | 20:AT:27:LYS:H      | 1.66                     | 0.42              |
| 22:AW:77:A:N6      | 35:BA:2422:A:O4'    | 2.52                     | 0.42              |
| 24:AY:182:ARG:HG3  | 24:AY:182:ARG:NH1   | 2.34                     | 0.42              |
| 24:AY:206:LEU:O    | 24:AY:209:ALA:HB3   | 2.19                     | 0.42              |
| 24:AY:327:PHE:HA   | 24:AY:375:GLY:O     | 2.19                     | 0.42              |
| 24:AY:395:PRO:HB2  | 24:AY:397:VAL:HG13  | 2.01                     | 0.42              |
| 24:AY:526:VAL:HG23 | 24:AY:565:VAL:O     | 2.18                     | 0.42              |
| 27:B2:38:GLN:HE21  | 27:B2:44:LEU:HB2    | 1.84                     | 0.42              |
| 29:B4:25:TYR:N     | 29:B4:25:TYR:CD1    | 2.86                     | 0.42              |
| 29:B4:29:PRO:HB2   | 29:B4:30:GLU:OE1    | 2.19                     | 0.42              |
| 19:AS:9:VAL:HG21   | 29:B4:53:GLU:CG     | 2.49                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 30:B5:44:THR:O     | 30:B5:51:TYR:CE1  | 2.70                     | 0.42              |
| 32:B7:33:ARG:HH11  | 32:B7:33:ARG:HB2  | 1.84                     | 0.42              |
| 33:B8:48:PHE:HB3   | 33:B8:49:VAL:H    | 1.46                     | 0.42              |
| 34:B9:29:ASN:N     | 34:B9:29:ASN:ND2  | 2.66                     | 0.42              |
| 35:BA:1128:A:C8    | 35:BA:2518:A:N6   | 2.87                     | 0.42              |
| 35:BA:1131:G:N3    | 35:BA:1132:A:C8   | 2.87                     | 0.42              |
| 35:BA:1204:A:H2    | 35:BA:1241:A:N1   | 2.17                     | 0.42              |
| 35:BA:811:U:O2     | 35:BA:1251:C:C6   | 2.71                     | 0.42              |
| 35:BA:1360:A:H5'   | 35:BA:1361:G:OP2  | 2.19                     | 0.42              |
| 35:BA:1888:G:N3    | 35:BA:1888:G:H5'  | 2.34                     | 0.42              |
| 35:BA:1973:G:H2'   | 35:BA:1974:C:C6   | 2.54                     | 0.42              |
| 35:BA:2089:U:O2'   | 35:BA:2090:G:H5'  | 2.19                     | 0.42              |
| 35:BA:2147:G:H2'   | 35:BA:2148:G:C4'  | 2.49                     | 0.42              |
| 35:BA:2389:G:H5''  | 35:BA:2390:U:O4'  | 2.19                     | 0.42              |
| 35:BA:245:G:O2'    | 35:BA:246:C:H5'   | 2.19                     | 0.42              |
| 35:BA:2604:U:H2'   | 35:BA:2605:U:H6   | 1.83                     | 0.42              |
| 35:BA:2839:G:H2'   | 35:BA:2840:C:H6   | 1.83                     | 0.42              |
| 35:BA:300:A:P      | 57:BY:97:ARG:HE   | 2.41                     | 0.42              |
| 35:BA:520:G:H2'    | 35:BA:521:G:C8    | 2.53                     | 0.42              |
| 32:B7:16:HIS:ND1   | 35:BA:684:G:OP1   | 2.51                     | 0.42              |
| 35:BA:811:U:O2     | 35:BA:1251:C:C5   | 2.72                     | 0.42              |
| 35:BA:817:C:O2'    | 35:BA:839:U:OP1   | 2.37                     | 0.42              |
| 35:BA:8:A:H2'      | 35:BA:9:U:C6      | 2.54                     | 0.42              |
| 37:BC:98:GLU:HA    | 37:BC:101:ILE:CD1 | 2.48                     | 0.42              |
| 40:BF:160:ASN:ND2  | 40:BF:161:GLU:N   | 2.67                     | 0.42              |
| 41:BG:145:THR:OG1  | 41:BG:146:TYR:N   | 2.52                     | 0.42              |
| 42:BH:136:ILE:HD12 | 42:BH:136:ILE:H   | 1.84                     | 0.42              |
| 43:BJ:118:UNK:N    | 43:BJ:121:UNK:O   | 2.52                     | 0.42              |
| 49:BQ:26:TYR:CD1   | 49:BQ:140:ALA:HB3 | 2.54                     | 0.42              |
| 49:BQ:52:VAL:HG12  | 49:BQ:53:ALA:N    | 2.33                     | 0.42              |
| 50:BR:13:HIS:O     | 50:BR:14:SER:C    | 2.56                     | 0.42              |
| 50:BR:21:TYR:N     | 50:BR:21:TYR:CD2  | 2.87                     | 0.42              |
| 51:BS:101:LEU:C    | 51:BS:101:LEU:CD1 | 2.87                     | 0.42              |
| 52:BT:16:ARG:HG3   | 52:BT:16:ARG:HH11 | 1.84                     | 0.42              |
| 53:BU:53:ARG:HG3   | 53:BU:57:PHE:HE1  | 1.84                     | 0.42              |
| 55:BW:13:SER:HB3   | 55:BW:16:LYS:HD2  | 2.00                     | 0.42              |
| 56:BX:28:PHE:N     | 56:BX:28:PHE:CD1  | 2.82                     | 0.42              |
| 1:CA:1277:C:H3'    | 1:CA:1277:C:C6    | 2.53                     | 0.42              |
| 1:CA:1296:C:H3'    | 1:CA:1297:C:H6    | 1.84                     | 0.42              |
| 1:CA:186:C:C2      | 1:CA:187:C:C5     | 3.07                     | 0.42              |
| 1:CA:202:U:H5'     | 1:CA:203:U:H5     | 1.84                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:316:G:C6     | 1:CA:338:A:C6      | 3.07                     | 0.42              |
| 1:CA:47:C:H6      | 1:CA:365:U:H2'     | 1.84                     | 0.42              |
| 1:CA:994:A:H2'    | 1:CA:994:A:N3      | 2.33                     | 0.42              |
| 2:CB:223:ILE:HG12 | 2:CB:226:ARG:HH22  | 1.79                     | 0.42              |
| 3:CC:43:LEU:C     | 3:CC:45:LYS:N      | 2.72                     | 0.42              |
| 3:CC:68:VAL:HG12  | 3:CC:70:VAL:HG23   | 2.00                     | 0.42              |
| 4:CD:140:VAL:HG12 | 4:CD:141:ARG:O     | 2.19                     | 0.42              |
| 4:CD:159:ARG:HG3  | 4:CD:159:ARG:NH1   | 2.33                     | 0.42              |
| 5:CE:145:LYS:HA   | 8:CH:107:LEU:HD21  | 2.01                     | 0.42              |
| 8:CH:99:GLU:O     | 8:CH:100:ILE:C     | 2.57                     | 0.42              |
| 9:CI:125:TYR:HD2  | 9:CI:126:SER:N     | 2.17                     | 0.42              |
| 10:CJ:40:LEU:HD23 | 10:CJ:40:LEU:H     | 1.81                     | 0.42              |
| 11:CK:21:ILE:CD1  | 11:CK:21:ILE:N     | 2.82                     | 0.42              |
| 16:CP:57:ARG:O    | 16:CP:58:TYR:C     | 2.57                     | 0.42              |
| 19:CS:41:VAL:CG2  | 19:CS:44:MET:HB2   | 2.37                     | 0.42              |
| 20:CT:81:LYS:C    | 20:CT:83:ARG:H     | 2.23                     | 0.42              |
| 24:CY:224:ASP:HB2 | 24:CY:227:ILE:HD12 | 2.01                     | 0.42              |
| 30:D5:3:LYS:HG2   | 35:DA:747:U:C4     | 2.54                     | 0.42              |
| 35:DA:1461:G:H2'  | 35:DA:1462:C:C6    | 2.53                     | 0.42              |
| 35:DA:1827:C:H2'  | 35:DA:1828:G:C5'   | 2.49                     | 0.42              |
| 35:DA:1941:C:C4   | 35:DA:1942:C:C4    | 3.06                     | 0.42              |
| 35:DA:200:U:C2'   | 35:DA:201:C:H5'    | 2.46                     | 0.42              |
| 35:DA:2020:A:N1   | 35:DA:2022:U:C2    | 2.87                     | 0.42              |
| 35:DA:2126:A:N1   | 35:DA:2162:G:O2'   | 2.46                     | 0.42              |
| 35:DA:2309:A:H2'  | 35:DA:2310:A:C5'   | 2.49                     | 0.42              |
| 35:DA:2460:U:H2'  | 35:DA:2460:U:O2    | 2.18                     | 0.42              |
| 35:DA:2489:G:C6   | 35:DA:2490:G:C6    | 3.07                     | 0.42              |
| 35:DA:1786:A:C2   | 35:DA:2606:C:H1'   | 2.54                     | 0.42              |
| 35:DA:2849:U:H1'  | 35:DA:2866:U:H6    | 1.84                     | 0.42              |
| 35:DA:460:A:H2'   | 35:DA:461:C:O4'    | 2.18                     | 0.42              |
| 35:DA:688:U:C4'   | 35:DA:1780:A:C2    | 3.01                     | 0.42              |
| 35:DA:68:G:H2'    | 35:DA:69:C:H6      | 1.84                     | 0.42              |
| 35:DA:729:G:O2'   | 35:DA:763:G:H4'    | 2.19                     | 0.42              |
| 38:DD:176:ARG:NH1 | 38:DD:176:ARG:CG   | 2.81                     | 0.42              |
| 38:DD:127:VAL:HA  | 38:DD:193:VAL:HG13 | 2.00                     | 0.42              |
| 35:DA:1902:C:C4'  | 38:DD:244:ARG:HB2  | 2.49                     | 0.42              |
| 38:DD:31:LYS:O    | 38:DD:33:LEU:N     | 2.51                     | 0.42              |
| 41:DG:168:GLU:O   | 41:DG:170:ARG:N    | 2.52                     | 0.42              |
| 41:DG:4:ASP:HA    | 41:DG:8:LYS:HG2    | 2.00                     | 0.42              |
| 42:DH:74:ASN:OD1  | 42:DH:138:LYS:HE3  | 2.19                     | 0.42              |
| 46:DN:60:ILE:HG22 | 46:DN:61:ARG:N     | 2.33                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 47:DO:24:VAL:O     | 47:DO:24:VAL:CG2  | 2.65                     | 0.42              |
| 47:DO:69:ILE:CD1   | 47:DO:77:ILE:HG23 | 2.41                     | 0.42              |
| 40:DF:116:ASP:OD2  | 48:DP:5:ASP:N     | 2.52                     | 0.42              |
| 49:DQ:12:GLN:HG2   | 49:DQ:73:PRO:HD2  | 2.01                     | 0.42              |
| 50:DR:13:HIS:O     | 50:DR:14:SER:C    | 2.57                     | 0.42              |
| 53:DU:59:ARG:CG    | 53:DU:59:ARG:HH11 | 2.24                     | 0.42              |
| 57:DY:14:LEU:HB2   | 57:DY:24:VAL:HG22 | 2.00                     | 0.42              |
| 1:AA:1371:G:C5     | 1:AA:1372:U:C5    | 3.07                     | 0.42              |
| 1:AA:333:G:O2'     | 1:AA:334:C:H5'    | 2.18                     | 0.42              |
| 1:AA:605:U:O2'     | 1:AA:606:G:H5'    | 2.19                     | 0.42              |
| 2:AB:178:ARG:HD2   | 8:AH:71:GLY:C     | 2.40                     | 0.42              |
| 2:AB:238:LEU:O     | 2:AB:239:VAL:C    | 2.57                     | 0.42              |
| 3:AC:47:LEU:HD21   | 3:AC:68:VAL:HG11  | 2.00                     | 0.42              |
| 4:AD:132:ARG:C     | 4:AD:132:ARG:HD2  | 2.39                     | 0.42              |
| 1:AA:1080:A:C5'    | 5:AE:16:THR:HG21  | 2.49                     | 0.42              |
| 8:AH:19:VAL:HG23   | 8:AH:21:LYS:HB2   | 2.01                     | 0.42              |
| 9:AI:105:ASP:OD1   | 9:AI:107:ARG:HD3  | 2.18                     | 0.42              |
| 10:AJ:31:GLY:O     | 10:AJ:32:ALA:C    | 2.58                     | 0.42              |
| 12:AL:83:VAL:HG12  | 12:AL:84:LEU:N    | 2.34                     | 0.42              |
| 13:AM:19:LEU:HA    | 13:AM:22:ILE:HD13 | 2.00                     | 0.42              |
| 13:AM:91:ARG:CD    | 13:AM:97:PRO:O    | 2.67                     | 0.42              |
| 15:AO:43:LEU:C     | 15:AO:45:VAL:H    | 2.21                     | 0.42              |
| 15:AO:64:ARG:CG    | 15:AO:64:ARG:HH11 | 2.32                     | 0.42              |
| 17:AQ:53:LEU:HD23  | 17:AQ:54:GLY:N    | 2.34                     | 0.42              |
| 18:AR:63:GLN:OE1   | 18:AR:63:GLN:HA   | 2.19                     | 0.42              |
| 20:AT:69:GLY:O     | 20:AT:73:HIS:NE2  | 2.52                     | 0.42              |
| 24:AY:191:ASP:O    | 24:AY:266:ASN:ND2 | 2.52                     | 0.42              |
| 24:AY:140:ASP:OD2  | 24:AY:265:LYS:HE2 | 2.19                     | 0.42              |
| 24:AY:289:ILE:HD12 | 24:AY:331:TYR:CE2 | 2.54                     | 0.42              |
| 27:B2:33:MET:HG2   | 27:B2:37:PHE:CE1  | 2.53                     | 0.42              |
| 29:B4:7:PRO:O      | 29:B4:8:LYS:HD2   | 2.19                     | 0.42              |
| 31:B6:26:ASN:O     | 31:B6:27:LYS:HB2  | 2.19                     | 0.42              |
| 35:BA:1131:G:C2    | 35:BA:1132:A:C5   | 3.07                     | 0.42              |
| 35:BA:1541:G:H4'   | 35:BA:1542:A:O4'  | 2.19                     | 0.42              |
| 35:BA:1815:A:H1'   | 35:BA:1817:G:C8   | 2.54                     | 0.42              |
| 35:BA:1932:A:H2'   | 35:BA:1933:G:O4'  | 2.19                     | 0.42              |
| 35:BA:2025:C:H2'   | 35:BA:2026:C:H6   | 1.84                     | 0.42              |
| 35:BA:2328:A:O5'   | 35:BA:2328:A:H8   | 2.02                     | 0.42              |
| 35:BA:2428:G:H5'   | 35:BA:2429:G:P    | 2.59                     | 0.42              |
| 35:BA:2511:U:H4'   | 39:BE:123:ALA:HB3 | 2.00                     | 0.42              |
| 35:BA:2537:U:H2'   | 35:BA:2538:C:H6   | 1.81                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:2579:C:H2'   | 35:BA:2580:U:O4'   | 2.20                     | 0.42              |
| 35:BA:272(J):C:H5' | 35:BA:274:G:OP2    | 2.18                     | 0.42              |
| 35:BA:2776:A:C6    | 35:BA:2782:G:H1'   | 2.53                     | 0.42              |
| 35:BA:2889:C:H2'   | 35:BA:2891:G:O4'   | 2.19                     | 0.42              |
| 35:BA:2809:A:C2    | 35:BA:2892:A:N3    | 2.87                     | 0.42              |
| 35:BA:772:C:O2'    | 35:BA:773:U:H5'    | 2.20                     | 0.42              |
| 35:BA:773:U:H2'    | 35:BA:774:A:H5'    | 2.00                     | 0.42              |
| 35:BA:685:A:C6     | 35:BA:774:A:C2     | 3.07                     | 0.42              |
| 35:BA:88:G:OP1     | 35:BA:90:U:C5      | 2.63                     | 0.42              |
| 35:BA:904:C:H2'    | 35:BA:905:U:C6     | 2.53                     | 0.42              |
| 35:BA:821:A:H2'    | 35:BA:946:G:H5''   | 2.00                     | 0.42              |
| 36:BB:81:G:O6      | 36:BB:96:U:O2      | 2.37                     | 0.42              |
| 37:BC:134:PRO:HB2  | 37:BC:135:ARG:HD2  | 2.01                     | 0.42              |
| 38:BD:267:SER:C    | 38:BD:270:ILE:HD11 | 2.40                     | 0.42              |
| 39:BE:144:ARG:HB3  | 39:BE:145:LYS:H    | 1.53                     | 0.42              |
| 40:BF:119:ARG:NH1  | 40:BF:119:ARG:HG2  | 2.33                     | 0.42              |
| 40:BF:20:LEU:HD13  | 40:BF:203:GLN:OE1  | 2.18                     | 0.42              |
| 42:BH:76:VAL:C     | 42:BH:78:GLY:H     | 2.21                     | 0.42              |
| 43:BJ:74:UNK:O     | 43:BJ:76:UNK:N     | 2.52                     | 0.42              |
| 49:BQ:76:LYS:HE2   | 49:BQ:77:LYS:O     | 2.18                     | 0.42              |
| 51:BS:89:ARG:CG    | 51:BS:92:TYR:CA    | 2.88                     | 0.42              |
| 52:BT:2:ASN:O      | 52:BT:4:GLY:N      | 2.51                     | 0.42              |
| 54:BV:19:LYS:HG2   | 54:BV:94:LEU:CB    | 2.48                     | 0.42              |
| 55:BW:50:VAL:HG13  | 55:BW:51:LEU:N     | 2.34                     | 0.42              |
| 49:BQ:63:LYS:NZ    | 58:BZ:175:VAL:HG21 | 2.34                     | 0.42              |
| 1:CA:1150:U:O4     | 1:CA:1151:A:N6     | 2.52                     | 0.42              |
| 1:CA:1386:G:O2'    | 1:CA:1387:G:H5'    | 2.19                     | 0.42              |
| 1:CA:1399:C:C2     | 1:CA:1401:G:C5     | 3.07                     | 0.42              |
| 1:CA:815:A:H62     | 1:CA:1509:C:H1'    | 1.83                     | 0.42              |
| 1:CA:193:C:C2      | 1:CA:194:C:C5      | 3.08                     | 0.42              |
| 1:CA:666:G:C2      | 1:CA:667:G:C8      | 3.08                     | 0.42              |
| 1:CA:963:G:H21     | 10:CJ:55:LYS:HD2   | 1.84                     | 0.42              |
| 2:CB:208:ILE:HA    | 2:CB:211:ILE:HD12  | 2.00                     | 0.42              |
| 2:CB:82:ARG:NH1    | 2:CB:82:ARG:HG3    | 2.33                     | 0.42              |
| 7:CG:144:MET:O     | 7:CG:147:ALA:HB3   | 2.19                     | 0.42              |
| 7:CG:61:VAL:O      | 7:CG:64:GLN:HB3    | 2.19                     | 0.42              |
| 9:CI:46:ALA:C      | 9:CI:47:LEU:HD12   | 2.39                     | 0.42              |
| 9:CI:51:ARG:HG3    | 9:CI:56:LEU:HD12   | 2.01                     | 0.42              |
| 9:CI:43:ALA:HA     | 9:CI:74:ILE:HD13   | 2.01                     | 0.42              |
| 12:CL:18:VAL:O     | 12:CL:19:ARG:CB    | 2.67                     | 0.42              |
| 13:CM:54:VAL:C     | 13:CM:56:LEU:N     | 2.72                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:CM:72:ALA:O     | 13:CM:75:ALA:N     | 2.53                     | 0.42              |
| 1:CA:582:U:OP1     | 15:CO:68:ARG:NH2   | 2.52                     | 0.42              |
| 22:CV:50:U:H2'     | 22:CV:51:C:C6      | 2.54                     | 0.42              |
| 24:CY:112:GLN:CG   | 24:CY:115:GLU:HB3  | 2.48                     | 0.42              |
| 24:CY:148:LEU:HD13 | 24:CY:151:ARG:NH1  | 2.29                     | 0.42              |
| 24:CY:309:LEU:HB3  | 24:CY:391:GLY:N    | 2.34                     | 0.42              |
| 24:CY:509:HIS:O    | 24:CY:510:VAL:CG2  | 2.67                     | 0.42              |
| 24:CY:538:TYR:HD1  | 24:CY:579:GLU:HA   | 1.84                     | 0.42              |
| 24:CY:539:ILE:CA   | 24:CY:542:VAL:HG12 | 2.48                     | 0.42              |
| 24:CY:678:GLU:HG2  | 24:CY:679:VAL:O    | 2.20                     | 0.42              |
| 61:CY:702:FUA:C23  | 61:CY:702:FUA:C12  | 2.84                     | 0.42              |
| 24:CY:69:VAL:CG2   | 24:CY:80:ASN:HB3   | 2.49                     | 0.42              |
| 25:D0:60:PHE:HE2   | 35:DA:2365:G:C4'   | 2.25                     | 0.42              |
| 27:D2:35:LEU:HD22  | 27:D2:50:ILE:CG1   | 2.49                     | 0.42              |
| 32:D7:46:VAL:HG12  | 32:D7:47:ARG:H     | 1.82                     | 0.42              |
| 35:DA:1146:C:H2'   | 35:DA:1146:C:O2    | 2.18                     | 0.42              |
| 35:DA:2336:A:H3'   | 35:DA:2337:G:H8    | 1.84                     | 0.42              |
| 35:DA:2290:G:H4'   | 35:DA:2381:C:O2'   | 2.19                     | 0.42              |
| 35:DA:2820:A:HO2'  | 35:DA:2821:A:P     | 2.42                     | 0.42              |
| 35:DA:2861:G:C4    | 35:DA:2862:G:C8    | 3.07                     | 0.42              |
| 35:DA:359:A:H3'    | 35:DA:360:G:C8     | 2.54                     | 0.42              |
| 35:DA:37:C:H2'     | 35:DA:37:C:O2      | 2.18                     | 0.42              |
| 36:DB:40:U:H3'     | 36:DB:41:U:H5''    | 2.00                     | 0.42              |
| 37:DC:65:LEU:HD21  | 37:DC:162:ILE:HD11 | 2.00                     | 0.42              |
| 35:DA:2820:A:H8    | 39:DE:191:PRO:HB3  | 1.84                     | 0.42              |
| 39:DE:82:ARG:HG3   | 39:DE:82:ARG:HH11  | 1.84                     | 0.42              |
| 40:DF:134:GLY:HA3  | 40:DF:165:ARG:NH1  | 2.34                     | 0.42              |
| 40:DF:7:TYR:CD2    | 40:DF:16:GLY:CA    | 3.00                     | 0.42              |
| 40:DF:63:LYS:HA    | 40:DF:76:GLY:O     | 2.19                     | 0.42              |
| 41:DG:53:LEU:HD12  | 41:DG:56:ALA:HB2   | 2.01                     | 0.42              |
| 42:DH:141:VAL:O    | 42:DH:142:GLY:C    | 2.57                     | 0.42              |
| 42:DH:146:ALA:O    | 42:DH:147:ASN:C    | 2.57                     | 0.42              |
| 42:DH:154:PRO:C    | 42:DH:156:ALA:H    | 2.17                     | 0.42              |
| 42:DH:52:VAL:HG12  | 42:DH:52:VAL:O     | 2.19                     | 0.42              |
| 44:DK:86:LYS:HZ3   | 44:DK:86:LYS:HB3   | 1.84                     | 0.42              |
| 47:DO:98:VAL:CG2   | 47:DO:118:ALA:HA   | 2.49                     | 0.42              |
| 48:DP:23:PRO:O     | 48:DP:29:LYS:O     | 2.37                     | 0.42              |
| 49:DQ:35:VAL:HG23  | 49:DQ:101:ARG:C    | 2.39                     | 0.42              |
| 50:DR:41:ALA:O     | 50:DR:43:GLU:N     | 2.53                     | 0.42              |
| 53:DU:53:ARG:CA    | 53:DU:56:ASP:OD2   | 2.62                     | 0.42              |
| 53:DU:98:LEU:HA    | 53:DU:101:ARG:O    | 2.19                     | 0.42              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:DZ:145:GLU:CG   | 58:DZ:146:ILE:H    | 2.32                     | 0.42              |
| 58:DZ:29:TYR:O     | 58:DZ:30:ASN:HB3   | 2.19                     | 0.42              |
| 58:DZ:77:ASP:C     | 58:DZ:78:LYS:HG2   | 2.40                     | 0.42              |
| 1:AA:1277:C:H3'    | 1:AA:1277:C:C6     | 2.54                     | 0.42              |
| 1:AA:182:U:O2      | 1:AA:182:U:H2'     | 2.19                     | 0.42              |
| 1:AA:267:C:H2'     | 1:AA:268:C:C6      | 2.48                     | 0.42              |
| 1:AA:452:A:H5'     | 16:AP:72:ARG:NH2   | 2.34                     | 0.42              |
| 1:AA:541:G:O2'     | 1:AA:542:G:H5'     | 2.19                     | 0.42              |
| 1:AA:893:C:O2'     | 1:AA:894:G:H5'     | 2.20                     | 0.42              |
| 3:AC:110:ASN:HD21  | 3:AC:140:ARG:HB3   | 1.84                     | 0.42              |
| 3:AC:87:LEU:O      | 3:AC:90:GLU:N      | 2.53                     | 0.42              |
| 4:AD:58:LEU:C      | 4:AD:58:LEU:CD2    | 2.86                     | 0.42              |
| 8:AH:74:PRO:O      | 8:AH:75:ARG:C      | 2.57                     | 0.42              |
| 9:AI:42:ARG:O      | 9:AI:44:VAL:N      | 2.52                     | 0.42              |
| 9:AI:90:PRO:HG2    | 9:AI:91:ASP:H      | 1.84                     | 0.42              |
| 10:AJ:29:ARG:CG    | 10:AJ:29:ARG:HH11  | 2.30                     | 0.42              |
| 1:AA:1061:G:H1'    | 10:AJ:56:HIS:CE1   | 2.53                     | 0.42              |
| 10:AJ:34:VAL:HG13  | 10:AJ:73:ASP:O     | 2.20                     | 0.42              |
| 13:AM:99:ARG:O     | 13:AM:100:GLY:O    | 2.37                     | 0.42              |
| 17:AQ:59:ILE:HG22  | 17:AQ:71:PHE:CD1   | 2.54                     | 0.42              |
| 20:AT:26:ASN:HD22  | 20:AT:27:LYS:N     | 2.17                     | 0.42              |
| 20:AT:43:LEU:O     | 20:AT:44:ALA:C     | 2.57                     | 0.42              |
| 24:AY:13:ARG:O     | 24:AY:79:ILE:HA    | 2.20                     | 0.42              |
| 24:AY:152:THR:C    | 24:AY:154:GLN:H    | 2.21                     | 0.42              |
| 24:AY:252:ASP:HB3  | 24:AY:254:LYS:NZ   | 2.34                     | 0.42              |
| 24:AY:289:ILE:HD12 | 24:AY:331:TYR:CZ   | 2.54                     | 0.42              |
| 24:AY:316:ILE:HD13 | 24:AY:316:ILE:N    | 2.34                     | 0.42              |
| 24:AY:456:GLU:HB2  | 24:AY:657:THR:HG21 | 2.01                     | 0.42              |
| 24:AY:21:ILE:HG23  | 24:AY:86:GLY:O     | 2.19                     | 0.42              |
| 27:B2:41:ILE:HD11  | 27:B2:44:LEU:CD1   | 2.38                     | 0.42              |
| 31:B6:9:LEU:HD21   | 31:B6:26:ASN:HD22  | 1.83                     | 0.42              |
| 35:BA:1019:U:N3    | 35:BA:1142(A):A:N6 | 2.66                     | 0.42              |
| 35:BA:1317:A:H2'   | 35:BA:1318:C:C6    | 2.54                     | 0.42              |
| 35:BA:2122:U:H4'   | 37:BC:167:ASP:HB3  | 2.01                     | 0.42              |
| 35:BA:2184:G:H2'   | 35:BA:2185:C:C6    | 2.54                     | 0.42              |
| 35:BA:2531:A:OP1   | 42:BH:177:GLY:O    | 2.38                     | 0.42              |
| 35:BA:2684:U:H2'   | 35:BA:2685:G:O4'   | 2.19                     | 0.42              |
| 35:BA:947:G:N3     | 35:BA:984:A:H2     | 2.18                     | 0.42              |
| 38:BD:158:ALA:O    | 38:BD:196:VAL:CG1  | 2.63                     | 0.42              |
| 39:BE:82:ARG:O     | 39:BE:83:ASP:C     | 2.57                     | 0.42              |
| 35:BA:322:A:C3'    | 40:BF:169:ASN:HD21 | 2.32                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 41:BG:10:LYS:O     | 41:BG:14:GLU:HB2  | 2.19                     | 0.42              |
| 42:BH:37:VAL:HG12  | 42:BH:38:SER:H    | 1.80                     | 0.42              |
| 44:BK:48:MET:HB2   | 44:BK:49:GLY:H    | 1.69                     | 0.42              |
| 47:BO:19:ILE:HD12  | 47:BO:41:ALA:CB   | 2.48                     | 0.42              |
| 47:BO:69:ILE:CD1   | 47:BO:77:ILE:HG23 | 2.36                     | 0.42              |
| 40:BF:116:ASP:OD2  | 48:BP:5:ASP:HB2   | 2.18                     | 0.42              |
| 51:BS:87:PHE:CG    | 51:BS:88:ASP:N    | 2.87                     | 0.42              |
| 52:BT:45:PHE:HE2   | 52:BT:74:ARG:HB2  | 1.81                     | 0.42              |
| 52:BT:8:LYS:O      | 52:BT:10:VAL:N    | 2.51                     | 0.42              |
| 57:BY:39:VAL:O     | 57:BY:40:GLU:CD   | 2.57                     | 0.42              |
| 57:BY:7:VAL:HB     | 57:BY:8:LYS:NZ    | 2.35                     | 0.42              |
| 57:BY:84:ARG:HG2   | 57:BY:85:VAL:H    | 1.84                     | 0.42              |
| 58:BZ:127:LYS:HZ3  | 58:BZ:164:ALA:HB2 | 1.84                     | 0.42              |
| 58:BZ:24:LEU:HD12  | 58:BZ:41:LEU:HD23 | 2.01                     | 0.42              |
| 1:CA:1054:C:C2'    | 1:CA:1054:C:O2    | 2.68                     | 0.42              |
| 1:CA:1221:G:OP1    | 1:CA:1320:C:N4    | 2.52                     | 0.42              |
| 1:CA:1509:C:C2'    | 1:CA:1510:U:H5'   | 2.49                     | 0.42              |
| 1:CA:767:A:H2'     | 1:CA:768:A:C8     | 2.55                     | 0.42              |
| 1:CA:963:G:HO2'    | 10:CJ:54:PHE:HZ   | 1.65                     | 0.42              |
| 3:CC:167:TRP:O     | 3:CC:168:ALA:CB   | 2.67                     | 0.42              |
| 3:CC:40:ARG:NH1    | 3:CC:40:ARG:HG3   | 2.34                     | 0.42              |
| 4:CD:4:TYR:CG      | 4:CD:5:ILE:N      | 2.85                     | 0.42              |
| 5:CE:6:PHE:N       | 5:CE:6:PHE:CD1    | 2.87                     | 0.42              |
| 9:CI:104:ARG:O     | 9:CI:105:ASP:N    | 2.52                     | 0.42              |
| 9:CI:84:ALA:O      | 9:CI:86:VAL:N     | 2.52                     | 0.42              |
| 10:CJ:40:LEU:CB    | 10:CJ:41:PRO:HD2  | 2.49                     | 0.42              |
| 13:CM:91:ARG:NH2   | 19:CS:81:ARG:NH2  | 2.67                     | 0.42              |
| 20:CT:89:ARG:HD2   | 20:CT:104:LEU:CD1 | 2.49                     | 0.42              |
| 22:CW:29:C:O2'     | 22:CW:30:G:H5'    | 2.19                     | 0.42              |
| 24:CY:181:LEU:HD21 | 24:CY:243:VAL:CG2 | 2.37                     | 0.42              |
| 24:CY:302:HIS:O    | 24:CY:304:ASP:N   | 2.49                     | 0.42              |
| 24:CY:342:TYR:O    | 24:CY:389:LEU:HA  | 2.19                     | 0.42              |
| 24:CY:553:GLY:H    | 24:CY:557:GLY:C   | 2.22                     | 0.42              |
| 24:CY:541:ALA:CB   | 24:CY:579:GLU:HG2 | 2.47                     | 0.42              |
| 26:D1:87:PRO:HG2   | 26:D1:88:LYS:H    | 1.85                     | 0.42              |
| 27:D2:14:ARG:HD3   | 27:D2:63:VAL:CG2  | 2.49                     | 0.42              |
| 29:D4:29:PRO:HB2   | 29:D4:30:GLU:OE1  | 2.19                     | 0.42              |
| 29:D4:5:ILE:HD13   | 29:D4:6:HIS:CD2   | 2.54                     | 0.42              |
| 35:DA:1186:G:H2'   | 35:DA:1187:G:H5'  | 2.01                     | 0.42              |
| 35:DA:1385:G:H4'   | 35:DA:1386:C:OP1  | 2.18                     | 0.42              |
| 35:DA:1415:U:H3    | 35:DA:1587:A:H61  | 1.66                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:143(A):C:H2' | 35:DA:143(A):C:O2  | 2.18                     | 0.42              |
| 35:DA:1530:C:H2'   | 35:DA:1531:C:H6    | 1.83                     | 0.42              |
| 35:DA:1710:C:H2'   | 35:DA:1711:C:C6    | 2.53                     | 0.42              |
| 35:DA:1947:C:C3'   | 35:DA:1948:G:H5''  | 2.50                     | 0.42              |
| 35:DA:2389:G:H5''  | 35:DA:2390:U:O4'   | 2.20                     | 0.42              |
| 35:DA:26:G:N1      | 35:DA:27:G:N2      | 2.67                     | 0.42              |
| 35:DA:329:G:H22    | 57:DY:19:LYS:HE3   | 1.83                     | 0.42              |
| 35:DA:594:U:H2'    | 35:DA:595:C:C6     | 2.54                     | 0.42              |
| 35:DA:615:G:OP2    | 40:DF:40:GLN:NE2   | 2.47                     | 0.42              |
| 35:DA:653:A:H5'    | 35:DA:654:A:P      | 2.58                     | 0.42              |
| 35:DA:805:G:H4'    | 35:DA:806:C:OP2    | 2.20                     | 0.42              |
| 36:DB:105:A:OP1    | 58:DZ:72:ARG:NH1   | 2.51                     | 0.42              |
| 37:DC:126:SER:C    | 37:DC:128:LEU:H    | 2.23                     | 0.42              |
| 37:DC:138:LEU:O    | 37:DC:139:PRO:C    | 2.57                     | 0.42              |
| 38:DD:85:ASP:OD2   | 38:DD:88:ARG:NH1   | 2.50                     | 0.42              |
| 39:DE:26:ILE:CG2   | 39:DE:196:VAL:HG21 | 2.47                     | 0.42              |
| 42:DH:94:TYR:HD1   | 42:DH:94:TYR:N     | 2.17                     | 0.42              |
| 43:DJ:45:UNK:C     | 43:DJ:47:UNK:H     | 2.31                     | 0.42              |
| 44:DK:10:LEU:HD11  | 44:DK:27:LEU:CD1   | 2.49                     | 0.42              |
| 44:DK:112:MET:HE1  | 44:DK:120:LEU:HD21 | 2.00                     | 0.42              |
| 46:DN:56:ASN:HA    | 46:DN:125:GLY:N    | 2.34                     | 0.42              |
| 46:DN:133:GLN:HG2  | 46:DN:134:ARG:H    | 1.83                     | 0.42              |
| 47:DO:10:VAL:HG21  | 47:DO:16:ALA:O     | 2.20                     | 0.42              |
| 40:DF:34:TRP:CB    | 48:DP:10:PRO:HB2   | 2.36                     | 0.42              |
| 48:DP:121:LYS:HB2  | 48:DP:123:LEU:HD21 | 2.01                     | 0.42              |
| 48:DP:66:GLY:O     | 48:DP:67:MET:CB    | 2.67                     | 0.42              |
| 50:DR:85:PRO:C     | 50:DR:87:TYR:N     | 2.73                     | 0.42              |
| 51:DS:47:THR:HG22  | 51:DS:49:VAL:O     | 2.19                     | 0.42              |
| 51:DS:87:PHE:CG    | 51:DS:88:ASP:N     | 2.87                     | 0.42              |
| 52:DT:35:LYS:HZ3   | 52:DT:41:ARG:HH11  | 1.64                     | 0.42              |
| 52:DT:89:VAL:C     | 52:DT:91:ARG:N     | 2.72                     | 0.42              |
| 53:DU:21:ALA:O     | 53:DU:22:LYS:C     | 2.57                     | 0.42              |
| 1:AA:1090:U:H4'    | 1:AA:1170:A:H2     | 1.85                     | 0.42              |
| 1:AA:1314:C:N4     | 19:AS:4:SER:N      | 2.67                     | 0.42              |
| 1:AA:1351:U:H5'    | 7:AG:33:ASP:OD1    | 2.20                     | 0.42              |
| 1:AA:1515:C:H2'    | 1:AA:1516:G:C8     | 2.54                     | 0.42              |
| 1:AA:394:G:H2'     | 1:AA:395:C:C6      | 2.55                     | 0.42              |
| 1:AA:437:U:H2'     | 1:AA:438:G:O4'     | 2.20                     | 0.42              |
| 1:AA:505:G:C6      | 1:AA:535:A:C2      | 3.07                     | 0.42              |
| 1:AA:1074:G:H4'    | 2:AB:104:ASN:HB2   | 2.01                     | 0.42              |
| 2:AB:24:TRP:HA     | 2:AB:190:THR:O     | 2.19                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:AB:204:ASN:HD21 | 2:AB:206:ASP:H    | 1.60                     | 0.42              |
| 3:AC:147:LYS:O    | 3:AC:203:PHE:HD2  | 2.02                     | 0.42              |
| 4:AD:127:THR:HG23 | 4:AD:147:ALA:HB3  | 2.01                     | 0.42              |
| 4:AD:190:ASP:HB3  | 4:AD:193:ASP:OD2  | 2.19                     | 0.42              |
| 8:AH:6:ILE:HG21   | 8:AH:85:ARG:NH1   | 2.34                     | 0.42              |
| 9:AI:126:SER:O    | 9:AI:127:LYS:HB3  | 2.20                     | 0.42              |
| 10:AJ:35:SER:O    | 10:AJ:36:GLY:O    | 2.37                     | 0.42              |
| 11:AK:120:ARG:NH1 | 11:AK:126:ARG:NE  | 2.67                     | 0.42              |
| 1:AA:539:A:OP2    | 12:AL:115:LYS:HE3 | 2.19                     | 0.42              |
| 12:AL:98:TYR:N    | 12:AL:98:TYR:CD1  | 2.86                     | 0.42              |
| 15:AO:3:ILE:O     | 15:AO:3:ILE:HG13  | 2.19                     | 0.42              |
| 1:AA:323:U:H5'    | 20:AT:23:ARG:HB2  | 2.00                     | 0.42              |
| 20:AT:64:ASP:OD1  | 20:AT:81:LYS:HD2  | 2.19                     | 0.42              |
| 22:AV:61:C:H2'    | 22:AV:62:C:H6     | 1.85                     | 0.42              |
| 22:AV:76:A:H4'    | 22:AV:76:A:OP1    | 2.19                     | 0.42              |
| 22:AW:37:U:H2'    | 22:AW:38:A:H8     | 1.84                     | 0.42              |
| 22:AW:73:A:H2'    | 22:AW:74:A:O4'    | 2.19                     | 0.42              |
| 24:AY:308:PRO:O   | 24:AY:333:GLY:N   | 2.52                     | 0.42              |
| 24:AY:416:LYS:CD  | 24:AY:417:THR:N   | 2.67                     | 0.42              |
| 24:AY:456:GLU:O   | 24:AY:457:LEU:C   | 2.58                     | 0.42              |
| 24:AY:90:PHE:HB2  | 24:AY:454:MET:CE  | 2.49                     | 0.42              |
| 28:B3:31:LEU:CD1  | 28:B3:32:GLN:HG2  | 2.33                     | 0.42              |
| 28:B3:35:ARG:HD3  | 28:B3:37:LEU:HD21 | 2.02                     | 0.42              |
| 29:B4:22:ILE:HG22 | 29:B4:24:THR:HG23 | 2.00                     | 0.42              |
| 35:BA:1209:G:H21  | 35:BA:1210:A:H62  | 1.66                     | 0.42              |
| 35:BA:143:G:H2'   | 35:BA:143(A):C:H6 | 1.84                     | 0.42              |
| 35:BA:1491:G:N3   | 35:BA:1491:G:H2'  | 2.34                     | 0.42              |
| 35:BA:1682:G:O2'  | 35:BA:1683:C:H5'  | 2.19                     | 0.42              |
| 35:BA:2012:G:O3'  | 55:BW:96:ILE:HG13 | 2.19                     | 0.42              |
| 35:BA:2154:G:C2   | 35:BA:2155:G:C4   | 3.08                     | 0.42              |
| 35:BA:2103:C:N4   | 35:BA:2186:G:H1   | 2.18                     | 0.42              |
| 35:BA:2665:A:H2'  | 35:BA:2666:C:O4'  | 2.19                     | 0.42              |
| 35:BA:512:G:O2'   | 35:BA:513:A:H8    | 2.02                     | 0.42              |
| 35:BA:611:C:H2'   | 35:BA:612:C:C6    | 2.54                     | 0.42              |
| 35:BA:893:C:H2'   | 35:BA:894:C:C6    | 2.54                     | 0.42              |
| 37:BC:196:ALA:O   | 37:BC:199:ALA:HB3 | 2.19                     | 0.42              |
| 37:BC:76:LEU:HD21 | 37:BC:104:ILE:CD1 | 2.48                     | 0.42              |
| 38:BD:96:HIS:CE1  | 38:BD:102:LYS:HE2 | 2.54                     | 0.42              |
| 38:BD:245:PRO:O   | 38:BD:246:PRO:O   | 2.37                     | 0.42              |
| 39:BE:45:THR:O    | 39:BE:46:ALA:CB   | 2.66                     | 0.42              |
| 41:BG:97:ASP:O    | 41:BG:101:ILE:CB  | 2.68                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:BG:56:ALA:HB1  | 41:BG:153:ARG:NH2 | 2.35                     | 0.42              |
| 41:BG:96:ARG:O    | 41:BG:97:ASP:CB   | 2.68                     | 0.42              |
| 42:BH:94:TYR:N    | 42:BH:94:TYR:HD1  | 2.17                     | 0.42              |
| 43:BJ:42:UNK:HA   | 43:BJ:45:UNK:CB   | 2.49                     | 0.42              |
| 46:BN:34:LEU:HD13 | 46:BN:34:LEU:HA   | 1.90                     | 0.42              |
| 46:BN:4:TYR:O     | 46:BN:5:VAL:C     | 2.57                     | 0.42              |
| 47:BO:14:THR:HG21 | 47:BO:86:ILE:HD13 | 2.02                     | 0.42              |
| 35:BA:662:G:P     | 48:BP:18:ARG:HD2  | 2.59                     | 0.42              |
| 50:BR:28:LEU:HA   | 50:BR:34:ILE:CG1  | 2.49                     | 0.42              |
| 50:BR:82:GLU:O    | 50:BR:85:PRO:HD2  | 2.19                     | 0.42              |
| 51:BS:48:LEU:N    | 51:BS:48:LEU:HD12 | 2.34                     | 0.42              |
| 51:BS:89:ARG:CG   | 51:BS:92:TYR:CB   | 2.96                     | 0.42              |
| 52:BT:67:SER:O    | 52:BT:68:TYR:HB2  | 2.20                     | 0.42              |
| 52:BT:70:VAL:HG12 | 52:BT:71:GLY:N    | 2.34                     | 0.42              |
| 53:BU:59:ARG:NH1  | 53:BU:59:ARG:HG2  | 2.29                     | 0.42              |
| 58:BZ:105:VAL:CG1 | 58:BZ:105:VAL:O   | 2.66                     | 0.42              |
| 58:BZ:115:GLY:HA2 | 58:BZ:177:PRO:CG  | 2.49                     | 0.42              |
| 58:BZ:52:SER:OG   | 58:BZ:53:ILE:N    | 2.52                     | 0.42              |
| 1:CA:1414:U:H2'   | 1:CA:1415:G:C8    | 2.54                     | 0.42              |
| 1:CA:189(B):C:C2  | 1:CA:189(J):G:C2  | 3.07                     | 0.42              |
| 1:CA:308:C:H2'    | 1:CA:309:G:C8     | 2.53                     | 0.42              |
| 1:CA:622:A:C8     | 1:CA:623:C:C6     | 3.07                     | 0.42              |
| 1:CA:658:G:H2'    | 1:CA:659:U:H6     | 1.83                     | 0.42              |
| 1:CA:690:G:H2'    | 1:CA:691:G:O4'    | 2.20                     | 0.42              |
| 1:CA:96:U:O2'     | 1:CA:97:G:H8      | 2.02                     | 0.42              |
| 2:CB:142:LEU:O    | 2:CB:146:GLN:HB2  | 2.19                     | 0.42              |
| 2:CB:170:GLU:C    | 2:CB:172:ILE:HD12 | 2.40                     | 0.42              |
| 3:CC:67:THR:HA    | 3:CC:102:ASN:HB2  | 2.01                     | 0.42              |
| 3:CC:78:GLY:CA    | 3:CC:83:ARG:HB3   | 2.50                     | 0.42              |
| 5:CE:33:VAL:HG12  | 5:CE:112:LEU:HD12 | 2.01                     | 0.42              |
| 6:CF:12:PRO:C     | 6:CF:14:LEU:H     | 2.23                     | 0.42              |
| 9:CI:95:LYS:NZ    | 9:CI:96:LEU:CD1   | 2.76                     | 0.42              |
| 10:CJ:32:ALA:HB1  | 10:CJ:75:ILE:CG1  | 2.48                     | 0.42              |
| 10:CJ:63:PHE:HB3  | 14:CN:58:LYS:CA   | 2.42                     | 0.42              |
| 13:CM:3:ARG:CA    | 13:CM:9:ILE:HG13  | 2.45                     | 0.42              |
| 19:CS:9:VAL:HG13  | 19:CS:39:THR:HB   | 2.02                     | 0.42              |
| 20:CT:61:SER:O    | 20:CT:63:ILE:N    | 2.52                     | 0.42              |
| 24:CY:293:THR:OG1 | 24:CY:297:GLU:HG2 | 2.20                     | 0.42              |
| 24:CY:308:PRO:O   | 24:CY:332:SER:CB  | 2.65                     | 0.42              |
| 24:CY:400:GLU:O   | 24:CY:402:ILE:CD1 | 2.64                     | 0.42              |
| 24:CY:527:ASN:ND2 | 24:CY:527:ASN:C   | 2.73                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:CY:625:ASN:C   | 24:CY:627:ARG:N   | 2.73                     | 0.42              |
| 25:D0:28:GLY:O    | 35:DA:923:C:O2'   | 2.31                     | 0.42              |
| 31:D6:11:LEU:HD13 | 31:D6:11:LEU:C    | 2.39                     | 0.42              |
| 33:D8:56:GLU:O    | 33:D8:59:LYS:CE   | 2.62                     | 0.42              |
| 34:D9:29:ASN:ND2  | 34:D9:32:HIS:CG   | 2.88                     | 0.42              |
| 35:DA:1052:C:C6   | 35:DA:1052:C:C3'  | 3.03                     | 0.42              |
| 35:DA:1150:C:O2'  | 35:DA:1151:G:H5'  | 2.18                     | 0.42              |
| 35:DA:1541:G:H4'  | 35:DA:1542:A:O4'  | 2.19                     | 0.42              |
| 35:DA:1349:A:N6   | 35:DA:1598:C:N4   | 2.67                     | 0.42              |
| 35:DA:1819:A:H4'  | 35:DA:1820:U:H5'' | 2.00                     | 0.42              |
| 35:DA:1821:A:H2'  | 35:DA:1822:G:C8   | 2.51                     | 0.42              |
| 35:DA:1952:A:C2   | 47:DO:22:ILE:HG23 | 2.55                     | 0.42              |
| 35:DA:2134:A:H1'  | 35:DA:2158:A:C2   | 2.54                     | 0.42              |
| 35:DA:2206:G:H21  | 35:DA:2207:G:H4'  | 1.84                     | 0.42              |
| 35:DA:2345:G:N7   | 35:DA:2372:G:C2   | 2.87                     | 0.42              |
| 33:D8:34:TRP:HB2  | 35:DA:2420:C:OP1  | 2.19                     | 0.42              |
| 35:DA:2428:G:C5'  | 35:DA:2429:G:OP1  | 2.66                     | 0.42              |
| 35:DA:1669:A:OP2  | 35:DA:2550:G:OP1  | 2.38                     | 0.42              |
| 32:D7:4:THR:O     | 35:DA:687:C:H5'   | 2.20                     | 0.42              |
| 35:DA:953:A:O2'   | 35:DA:954:G:H5'   | 2.20                     | 0.42              |
| 36:DB:114:C:H2'   | 36:DB:115:G:H8    | 1.84                     | 0.42              |
| 36:DB:74:U:C2'    | 36:DB:75:G:H5'    | 2.49                     | 0.42              |
| 39:DE:51:PHE:HD1  | 39:DE:52:LEU:HD12 | 1.83                     | 0.42              |
| 39:DE:51:PHE:O    | 39:DE:74:PRO:HB3  | 2.20                     | 0.42              |
| 39:DE:50:GLY:CA   | 39:DE:74:PRO:HG3  | 2.50                     | 0.42              |
| 40:DF:184:TYR:O   | 40:DF:188:ARG:HG2 | 2.19                     | 0.42              |
| 41:DG:13:GLU:O    | 41:DG:14:GLU:HB2  | 2.20                     | 0.42              |
| 42:DH:94:TYR:O    | 42:DH:95:ARG:HB3  | 2.19                     | 0.42              |
| 46:DN:15:LEU:HD13 | 46:DN:15:LEU:C    | 2.39                     | 0.42              |
| 46:DN:38:HIS:C    | 53:DU:67:ALA:HB1  | 2.39                     | 0.42              |
| 47:DO:13:ASN:ND2  | 47:DO:97:ARG:HB2  | 2.34                     | 0.42              |
| 49:DQ:136:ALA:C   | 49:DQ:138:ASP:H   | 2.20                     | 0.42              |
| 49:DQ:25:ASP:HA   | 49:DQ:100:GLY:O   | 2.18                     | 0.42              |
| 51:DS:49:VAL:CG1  | 51:DS:50:SER:N    | 2.81                     | 0.42              |
| 52:DT:102:ILE:O   | 52:DT:103:ARG:C   | 2.57                     | 0.42              |
| 46:DN:2:LYS:HE2   | 53:DU:95:LEU:HD21 | 2.02                     | 0.42              |
| 55:DW:68:ARG:HA   | 55:DW:110:LYS:CG  | 2.48                     | 0.42              |
| 56:DX:27:THR:HB   | 56:DX:80:ILE:CG2  | 2.45                     | 0.42              |
| 57:DY:86:ARG:CB   | 57:DY:88:LYS:HZ1  | 2.30                     | 0.42              |
| 58:DZ:14:LYS:O    | 58:DZ:18:LEU:CD1  | 2.67                     | 0.42              |
| 58:DZ:27:VAL:O    | 58:DZ:87:ASP:HA   | 2.19                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:DQ:135:ASP:CG   | 58:DZ:49:ARG:NH1   | 2.73                     | 0.42              |
| 1:AA:309:G:H1'     | 1:AA:608:A:H2      | 1.81                     | 0.42              |
| 1:AA:312:C:H2'     | 1:AA:313:A:C8      | 2.55                     | 0.42              |
| 1:AA:961:U:OP2     | 1:AA:1223:C:C4'    | 2.67                     | 0.42              |
| 2:AB:17:PHE:O      | 2:AB:18:GLY:O      | 2.36                     | 0.42              |
| 2:AB:55:PHE:HE1    | 2:AB:218:ALA:HA    | 1.84                     | 0.42              |
| 4:AD:61:LYS:HG3    | 4:AD:203:VAL:HG13  | 2.01                     | 0.42              |
| 5:AE:144:THR:C     | 5:AE:146:ALA:N     | 2.70                     | 0.42              |
| 7:AG:65:ALA:HB2    | 7:AG:128:ALA:HB2   | 2.02                     | 0.42              |
| 9:AI:42:ARG:O      | 9:AI:43:ALA:C      | 2.57                     | 0.42              |
| 9:AI:84:ALA:O      | 9:AI:86:VAL:N      | 2.52                     | 0.42              |
| 10:AJ:30:SER:HA    | 10:AJ:80:LYS:CE    | 2.49                     | 0.42              |
| 11:AK:126:ARG:O    | 11:AK:127:LYS:C    | 2.57                     | 0.42              |
| 24:AY:122:TRP:O    | 24:AY:124:GLN:N    | 2.51                     | 0.42              |
| 24:AY:238:THR:HG22 | 24:AY:241:GLU:CB   | 2.49                     | 0.42              |
| 24:AY:335:LEU:CD2  | 24:AY:355:LEU:HD11 | 2.49                     | 0.42              |
| 24:AY:97:SER:O     | 24:AY:100:VAL:CG1  | 2.67                     | 0.42              |
| 25:B0:28:GLY:O     | 35:BA:923:C:O2'    | 2.34                     | 0.42              |
| 28:B3:6:VAL:HG23   | 28:B3:6:VAL:O      | 2.18                     | 0.42              |
| 32:B7:46:VAL:CG1   | 32:B7:47:ARG:H     | 2.33                     | 0.42              |
| 33:B8:56:GLU:O     | 33:B8:59:LYS:CE    | 2.65                     | 0.42              |
| 35:BA:1342:A:C2    | 35:BA:1345:C:C5    | 3.08                     | 0.42              |
| 35:BA:1433:U:H1'   | 35:BA:1561:G:N2    | 2.34                     | 0.42              |
| 35:BA:1539:G:N1    | 35:BA:1540:U:O2    | 2.52                     | 0.42              |
| 35:BA:1478:G:O2'   | 35:BA:1558:A:C2    | 2.72                     | 0.42              |
| 35:BA:1430:C:H42   | 35:BA:1563:G:H1    | 1.67                     | 0.42              |
| 35:BA:1609:A:H1'   | 35:BA:1616:A:C1'   | 2.49                     | 0.42              |
| 35:BA:1960:A:H8    | 35:BA:1960:A:H5''  | 1.85                     | 0.42              |
| 35:BA:562:U:C4     | 35:BA:2036:C:H1'   | 2.55                     | 0.42              |
| 35:BA:2298:A:H2'   | 35:BA:2299:G:O4'   | 2.20                     | 0.42              |
| 35:BA:2341:G:H2'   | 35:BA:2342:C:C6    | 2.54                     | 0.42              |
| 35:BA:2693:A:H2'   | 35:BA:2694:G:H8    | 1.85                     | 0.42              |
| 35:BA:2713:A:H4'   | 35:BA:2713:A:OP2   | 2.19                     | 0.42              |
| 35:BA:2849:U:H4'   | 35:BA:2868:A:C2    | 2.54                     | 0.42              |
| 35:BA:483:A:C2     | 35:BA:484:C:C1'    | 3.03                     | 0.42              |
| 35:BA:799:G:C3'    | 35:BA:800:A:H5''   | 2.46                     | 0.42              |
| 36:BB:18:G:H2'     | 36:BB:19:G:C8      | 2.51                     | 0.42              |
| 36:BB:40:U:H3'     | 36:BB:41:U:H5''    | 2.00                     | 0.42              |
| 37:BC:11:LEU:C     | 37:BC:13:GLU:H     | 2.22                     | 0.42              |
| 37:BC:225:ILE:C    | 37:BC:225:ILE:HD12 | 2.40                     | 0.42              |
| 38:BD:112:GLN:HB2  | 38:BD:115:GLN:HE21 | 1.84                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:1814:G:C4'   | 38:BD:51:VAL:HG21  | 2.49                     | 0.42              |
| 39:BE:31:CYS:HA    | 39:BE:32:PRO:HD3   | 1.83                     | 0.42              |
| 39:BE:50:GLY:CA    | 39:BE:74:PRO:HG3   | 2.49                     | 0.42              |
| 40:BF:116:ASP:OD2  | 48:BP:5:ASP:N      | 2.52                     | 0.42              |
| 41:BG:53:LEU:HD12  | 41:BG:56:ALA:CB    | 2.50                     | 0.42              |
| 41:BG:39:ILE:HG12  | 41:BG:92:VAL:HG22  | 2.01                     | 0.42              |
| 42:BH:43:VAL:CG1   | 42:BH:51:ARG:O     | 2.68                     | 0.42              |
| 42:BH:94:TYR:O     | 42:BH:95:ARG:HB3   | 2.18                     | 0.42              |
| 44:BK:103:GLN:C    | 44:BK:106:GLU:HG2  | 2.39                     | 0.42              |
| 48:BP:144:GLU:N    | 48:BP:145:PRO:HD3  | 2.34                     | 0.42              |
| 48:BP:5:ASP:OD2    | 48:BP:9:ASN:ND2    | 2.51                     | 0.42              |
| 49:BQ:70:PRO:HA    | 49:BQ:95:ALA:HB2   | 2.01                     | 0.42              |
| 35:BA:1453:U:OP1   | 50:BR:63:ARG:NH2   | 2.52                     | 0.42              |
| 50:BR:82:GLU:O     | 50:BR:84:ALA:N     | 2.52                     | 0.42              |
| 55:BW:79:GLY:C     | 55:BW:100:THR:CG2  | 2.87                     | 0.42              |
| 56:BX:77:LYS:O     | 56:BX:77:LYS:HG2   | 2.19                     | 0.42              |
| 58:BZ:109:ALA:O    | 58:BZ:111:VAL:N    | 2.52                     | 0.42              |
| 58:BZ:111:VAL:O    | 58:BZ:112:ARG:CB   | 2.68                     | 0.42              |
| 1:CA:1000:U:H6     | 1:CA:1000:U:H3'    | 1.84                     | 0.42              |
| 1:CA:178:C:C2'     | 1:CA:179:A:H5'     | 2.49                     | 0.42              |
| 1:CA:555:C:H2'     | 1:CA:556:C:H6      | 1.84                     | 0.42              |
| 2:CB:204:ASN:ND2   | 2:CB:207:ALA:H     | 2.17                     | 0.42              |
| 4:CD:91:SER:O      | 4:CD:92:VAL:C      | 2.56                     | 0.42              |
| 5:CE:150:ARG:HB2   | 5:CE:150:ARG:CZ    | 2.49                     | 0.42              |
| 7:CG:23:VAL:HG13   | 7:CG:43:PHE:CE2    | 2.54                     | 0.42              |
| 9:CI:43:ALA:O      | 9:CI:45:ALA:N      | 2.53                     | 0.42              |
| 12:CL:105:TYR:CD2  | 12:CL:105:TYR:N    | 2.87                     | 0.42              |
| 1:CA:617:G:H4'     | 16:CP:44:THR:O     | 2.19                     | 0.42              |
| 17:CQ:51:TYR:CZ    | 17:CQ:73:VAL:HG11  | 2.54                     | 0.42              |
| 24:CY:268:GLY:HA2  | 24:CY:271:LEU:HD12 | 2.02                     | 0.42              |
| 24:CY:31:ARG:HA    | 24:CY:31:ARG:HD3   | 1.84                     | 0.42              |
| 24:CY:351:ARG:O    | 24:CY:351:ARG:HG3  | 2.18                     | 0.42              |
| 24:CY:510:VAL:HG13 | 24:CY:569:ASP:O    | 2.19                     | 0.42              |
| 24:CY:610:VAL:CG2  | 24:CY:643:ILE:HB   | 2.49                     | 0.42              |
| 24:CY:685:GLU:HA   | 24:CY:688:ILE:HD13 | 2.02                     | 0.42              |
| 25:D0:37:LEU:N     | 25:D0:59:LEU:O     | 2.49                     | 0.42              |
| 26:D1:84:GLY:O     | 26:D1:86:SER:OG    | 2.35                     | 0.42              |
| 27:D2:27:GLU:O     | 27:D2:28:LYS:C     | 2.58                     | 0.42              |
| 30:D5:44:THR:CG2   | 30:D5:45:VAL:N     | 2.79                     | 0.42              |
| 33:D8:32:LEU:H     | 33:D8:32:LEU:CD2   | 2.32                     | 0.42              |
| 35:DA:1062:G:H22   | 35:DA:1077:A:H1'   | 1.85                     | 0.42              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 35:DA:1276:A:C1'    | 50:DR:16:HIS:HE1    | 2.31                     | 0.42              |
| 35:DA:1493:C:H4'    | 35:DA:1494:A:OP1    | 2.19                     | 0.42              |
| 35:DA:1502:C:H2'    | 35:DA:1503:U:C6     | 2.54                     | 0.42              |
| 35:DA:1509(B):A:H2' | 35:DA:1510:G:C8     | 2.55                     | 0.42              |
| 35:DA:1433:U:H1'    | 35:DA:1561:G:N2     | 2.34                     | 0.42              |
| 35:DA:1632:A:C5     | 35:DA:1633:G:C6     | 3.08                     | 0.42              |
| 35:DA:1635:G:H2'    | 35:DA:1636:C:H6     | 1.84                     | 0.42              |
| 35:DA:1826:G:H2'    | 35:DA:1827:C:H6     | 1.85                     | 0.42              |
| 35:DA:1858:G:OP2    | 35:DA:1858:G:H8     | 2.03                     | 0.42              |
| 35:DA:2078:C:C4     | 35:DA:2079:U:C4     | 3.07                     | 0.42              |
| 22:CW:20:G:C4       | 35:DA:2169:A:C2     | 3.08                     | 0.42              |
| 35:DA:271(M):G:C2'  | 35:DA:271(N):U:H5'' | 2.49                     | 0.42              |
| 35:DA:2794:C:N4     | 35:DA:2801(A):A:H61 | 2.14                     | 0.42              |
| 35:DA:654(B):C:H2'  | 35:DA:654(C):G:C8   | 2.55                     | 0.42              |
| 35:DA:86:C:H4'      | 35:DA:104:U:O2      | 2.19                     | 0.42              |
| 35:DA:975:C:H4'     | 35:DA:975:C:OP2     | 2.19                     | 0.42              |
| 35:DA:987:G:H2'     | 35:DA:988:A:O4'     | 2.19                     | 0.42              |
| 35:DA:918:A:H1'     | 36:DB:80:U:O2'      | 2.19                     | 0.42              |
| 37:DC:225:ILE:C     | 37:DC:225:ILE:HD12  | 2.39                     | 0.42              |
| 38:DD:155:LEU:CD1   | 38:DD:155:LEU:N     | 2.82                     | 0.42              |
| 38:DD:4:LYS:NZ      | 38:DD:20:ASP:HA     | 2.34                     | 0.42              |
| 38:DD:85:ASP:CG     | 38:DD:88:ARG:HG2    | 2.40                     | 0.42              |
| 35:DA:1657:C:H4'    | 39:DE:133:LYS:HG2   | 2.02                     | 0.42              |
| 40:DF:118:ALA:O     | 40:DF:121:GLY:N     | 2.51                     | 0.42              |
| 40:DF:198:ALA:HA    | 40:DF:201:VAL:HG12  | 2.00                     | 0.42              |
| 42:DH:70:THR:C      | 42:DH:72:ILE:N      | 2.72                     | 0.42              |
| 42:DH:83:TYR:HB3    | 42:DH:134:SER:CA    | 2.40                     | 0.42              |
| 43:DJ:32:UNK:C      | 43:DJ:33:UNK:O      | 2.67                     | 0.42              |
| 43:DJ:35:UNK:C      | 43:DJ:37:UNK:H      | 2.32                     | 0.42              |
| 43:DJ:95:UNK:O      | 43:DJ:97:UNK:N      | 2.52                     | 0.42              |
| 48:DP:110:TYR:O     | 48:DP:111:ARG:O     | 2.38                     | 0.42              |
| 48:DP:98:GLU:H      | 48:DP:101:VAL:HG13  | 1.83                     | 0.42              |
| 50:DR:12:ARG:CG     | 50:DR:12:ARG:NH1    | 2.81                     | 0.42              |
| 53:DU:83:LEU:CD1    | 53:DU:113:ALA:HB2   | 2.49                     | 0.42              |
| 55:DW:72:LYS:H      | 55:DW:107:LEU:HA    | 1.85                     | 0.42              |
| 55:DW:61:ASN:HA     | 55:DW:61:ASN:HD22   | 1.62                     | 0.42              |
| 56:DX:63:LYS:HB3    | 56:DX:72:LYS:HG2    | 2.01                     | 0.42              |
| 57:DY:88:LYS:HE2    | 57:DY:93:GLY:HA3    | 2.00                     | 0.42              |
| 58:DZ:14:LYS:HB2    | 58:DZ:17:ALA:HB3    | 2.01                     | 0.42              |
| 36:DB:105:A:P       | 58:DZ:72:ARG:HH12   | 2.42                     | 0.42              |
| 1:AA:1104:G:O2'     | 1:AA:1105:A:H5'     | 2.20                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1122:U:H2'    | 1:AA:1123:A:H5'    | 2.01                     | 0.42              |
| 1:AA:1338:G:H2'    | 1:AA:1339:A:C8     | 2.55                     | 0.42              |
| 1:AA:1399:C:C2     | 1:AA:1401:G:C5     | 3.08                     | 0.42              |
| 1:AA:28:G:O2'      | 1:AA:296:U:OP1     | 2.35                     | 0.42              |
| 1:AA:499:A:O2'     | 1:AA:500:G:C8      | 2.64                     | 0.42              |
| 1:AA:745:C:H2'     | 1:AA:746:A:C8      | 2.54                     | 0.42              |
| 1:AA:954:G:H2'     | 1:AA:955:U:H6      | 1.83                     | 0.42              |
| 2:AB:52:GLU:O      | 2:AB:56:ARG:HG2    | 2.20                     | 0.42              |
| 3:AC:123:GLN:HB3   | 3:AC:128:PHE:CD2   | 2.44                     | 0.42              |
| 3:AC:127:ARG:NH1   | 3:AC:127:ARG:HG2   | 2.34                     | 0.42              |
| 4:AD:129:ASN:N     | 4:AD:129:ASN:ND2   | 2.68                     | 0.42              |
| 7:AG:118:VAL:O     | 7:AG:121:ALA:HB3   | 2.20                     | 0.42              |
| 9:AI:16:ARG:O      | 9:AI:63:ILE:HG23   | 2.20                     | 0.42              |
| 11:AK:91:ARG:O     | 11:AK:91:ARG:HG2   | 2.20                     | 0.42              |
| 13:AM:19:LEU:H     | 13:AM:19:LEU:CD2   | 2.32                     | 0.42              |
| 6:AF:100:ASN:O     | 18:AR:28:GLU:HG2   | 2.18                     | 0.42              |
| 19:AS:9:VAL:C      | 19:AS:11:VAL:N     | 2.73                     | 0.42              |
| 24:AY:260:LEU:O    | 24:AY:268:GLY:HA3  | 2.19                     | 0.42              |
| 24:AY:329:ARG:HG3  | 24:AY:331:TYR:CZ   | 2.54                     | 0.42              |
| 24:AY:442:THR:HG23 | 24:AY:447:GLY:O    | 2.19                     | 0.42              |
| 61:AY:702:FUA:C15  | 61:AY:702:FUA:H323 | 2.49                     | 0.42              |
| 25:B0:51:VAL:HG12  | 25:B0:59:LEU:HD22  | 2.02                     | 0.42              |
| 27:B2:47:ASN:O     | 27:B2:49:LYS:N     | 2.53                     | 0.42              |
| 30:B5:42:PRO:O     | 30:B5:43:HIS:HB2   | 2.20                     | 0.42              |
| 31:B6:11:LEU:CB    | 31:B6:26:ASN:HD21  | 2.32                     | 0.42              |
| 31:B6:8:LYS:HZ1    | 35:BA:2285:C:H5    | 1.58                     | 0.42              |
| 32:B7:27:GLY:HA2   | 32:B7:30:VAL:CG2   | 2.50                     | 0.42              |
| 33:B8:37:SER:O     | 33:B8:38:GLY:C     | 2.56                     | 0.42              |
| 35:BA:1265:A:H5'   | 35:BA:1267:U:C1'   | 2.46                     | 0.42              |
| 35:BA:1858:G:OP2   | 35:BA:1858:G:H8    | 2.02                     | 0.42              |
| 35:BA:201:C:C5     | 35:BA:202:U:C5     | 3.08                     | 0.42              |
| 35:BA:2078:C:C4    | 35:BA:2079:U:C4    | 3.08                     | 0.42              |
| 35:BA:2126:A:H1'   | 35:BA:2127:G:O4'   | 2.20                     | 0.42              |
| 35:BA:2206:G:H21   | 35:BA:2207:G:H4'   | 1.84                     | 0.42              |
| 35:BA:2422:A:H8    | 35:BA:2422:A:H3'   | 1.84                     | 0.42              |
| 35:BA:2552:U:H2'   | 35:BA:2554:U:H5''  | 2.01                     | 0.42              |
| 35:BA:27:G:H1'     | 35:BA:513:A:H62    | 1.84                     | 0.42              |
| 35:BA:294:A:N6     | 35:BA:345:A:H1'    | 2.35                     | 0.42              |
| 35:BA:868:U:C4     | 35:BA:869:G:N7     | 2.88                     | 0.42              |
| 36:BB:30:C:OP2     | 51:BS:32:LEU:HD21  | 2.20                     | 0.42              |
| 37:BC:117:THR:O    | 37:BC:120:VAL:HG22 | 2.19                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 37:BC:7:ARG:O     | 37:BC:11:LEU:HG    | 2.20                     | 0.42              |
| 37:BC:78:ILE:HG21 | 37:BC:124:VAL:CG2  | 2.49                     | 0.42              |
| 40:BF:157:VAL:HA  | 40:BF:176:LEU:O    | 2.18                     | 0.42              |
| 40:BF:83:PHE:O    | 40:BF:84:VAL:C     | 2.57                     | 0.42              |
| 42:BH:18:GLU:CB   | 42:BH:25:LYS:HB2   | 2.43                     | 0.42              |
| 44:BK:93:ARG:HD2  | 44:BK:93:ARG:O     | 2.20                     | 0.42              |
| 35:BA:1006:C:O2'  | 46:BN:106:MET:HB3  | 2.18                     | 0.42              |
| 46:BN:130:HIS:O   | 46:BN:130:HIS:CG   | 2.73                     | 0.42              |
| 46:BN:35:ARG:HB3  | 46:BN:42:TRP:CZ3   | 2.55                     | 0.42              |
| 47:BO:31:LYS:HB3  | 47:BO:32:TYR:CE1   | 2.54                     | 0.42              |
| 47:BO:88:ASN:O    | 47:BO:90:GLN:N     | 2.53                     | 0.42              |
| 50:BR:24:GLN:HB2  | 50:BR:44:LEU:HD23  | 2.01                     | 0.42              |
| 57:BY:103:GLY:O   | 57:BY:105:ALA:N    | 2.52                     | 0.42              |
| 1:CA:1483:A:H2'   | 1:CA:1484:C:O4'    | 2.19                     | 0.42              |
| 1:CA:201:C:C3'    | 1:CA:202:U:H5''    | 2.50                     | 0.42              |
| 1:CA:238:G:P      | 17:CQ:25:ARG:HH22  | 2.43                     | 0.42              |
| 1:CA:322:C:H41    | 1:CA:328:C:H6      | 1.66                     | 0.42              |
| 1:CA:356:A:H2'    | 1:CA:357:G:H8      | 1.85                     | 0.42              |
| 2:CB:97:TRP:CZ3   | 2:CB:173:ALA:HA    | 2.54                     | 0.42              |
| 3:CC:137:ALA:HA   | 3:CC:140:ARG:HH22  | 1.83                     | 0.42              |
| 3:CC:155:GLY:O    | 3:CC:156:ARG:CB    | 2.67                     | 0.42              |
| 4:CD:102:ASP:HA   | 4:CD:121:VAL:HG21  | 2.00                     | 0.42              |
| 5:CE:142:LEU:O    | 5:CE:143:ARG:CD    | 2.67                     | 0.42              |
| 5:CE:7:GLU:HB3    | 5:CE:35:GLY:O      | 2.20                     | 0.42              |
| 5:CE:82:VAL:HG21  | 5:CE:138:ALA:CA    | 2.41                     | 0.42              |
| 7:CG:153:HIS:CE1  | 11:CK:58:PRO:HD2   | 2.55                     | 0.42              |
| 7:CG:88:PRO:HG2   | 7:CG:88:PRO:O      | 2.20                     | 0.42              |
| 8:CH:97:VAL:HG13  | 8:CH:98:LYS:N      | 2.34                     | 0.42              |
| 9:CI:11:LYS:O     | 9:CI:12:GLU:HB2    | 2.20                     | 0.42              |
| 10:CJ:32:ALA:CB   | 10:CJ:76:ASN:HB3   | 2.49                     | 0.42              |
| 12:CL:91:LYS:HE2  | 12:CL:91:LYS:HB2   | 1.71                     | 0.42              |
| 13:CM:19:LEU:H    | 13:CM:19:LEU:CD2   | 2.32                     | 0.42              |
| 15:CO:69:TYR:CZ   | 15:CO:73:GLU:HG3   | 2.54                     | 0.42              |
| 16:CP:9:PHE:HE2   | 16:CP:18:ARG:HD2   | 1.83                     | 0.42              |
| 17:CQ:52:LYS:N    | 17:CQ:52:LYS:HD2   | 2.20                     | 0.42              |
| 19:CS:35:SER:C    | 19:CS:37:ARG:H     | 2.22                     | 0.42              |
| 22:CV:74:C:H2'    | 22:CV:75:C:C5'     | 2.49                     | 0.42              |
| 22:CW:73:A:C2'    | 22:CW:74:A:O5'     | 2.68                     | 0.42              |
| 24:CY:409:ILE:HA  | 24:CY:409:ILE:HD13 | 1.82                     | 0.42              |
| 24:CY:15:ILE:O    | 24:CY:81:ILE:HG23  | 2.20                     | 0.42              |
| 25:D0:49:LYS:HG3  | 25:D0:80:HIS:ND1   | 2.34                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:D1:53:VAL:HG11  | 26:D1:90:ILE:HG21  | 2.02                     | 0.42              |
| 33:D8:39:LYS:HE3   | 35:DA:2365:G:O6    | 2.19                     | 0.42              |
| 34:D9:16:VAL:O     | 35:DA:1033:U:H5    | 2.03                     | 0.42              |
| 35:DA:1133:U:O2    | 35:DA:1137:G:C5'   | 2.68                     | 0.42              |
| 35:DA:1142(A):A:C6 | 35:DA:1144:G:C5    | 3.07                     | 0.42              |
| 35:DA:1362:C:H2'   | 35:DA:1363:C:C6    | 2.55                     | 0.42              |
| 35:DA:1478:G:O2'   | 35:DA:1558:A:C2    | 2.72                     | 0.42              |
| 35:DA:1771:C:H2'   | 35:DA:1772:G:H8    | 1.85                     | 0.42              |
| 35:DA:1782:C:O5'   | 35:DA:1782:C:H6    | 2.02                     | 0.42              |
| 35:DA:1803:A:C8    | 35:DA:1804:C:C5    | 3.07                     | 0.42              |
| 35:DA:1805:U:H2'   | 35:DA:1806:C:C6    | 2.55                     | 0.42              |
| 35:DA:2033:A:O2'   | 35:DA:2034:U:P     | 2.78                     | 0.42              |
| 35:DA:2147:G:H2'   | 35:DA:2148:G:C4'   | 2.50                     | 0.42              |
| 35:DA:2553:G:H2'   | 35:DA:2554:U:C4'   | 2.49                     | 0.42              |
| 35:DA:2578:G:N2    | 35:DA:2579:C:C2    | 2.88                     | 0.42              |
| 35:DA:349:G:C2'    | 35:DA:350:U:H5'    | 2.50                     | 0.42              |
| 35:DA:696:G:C2     | 35:DA:767:U:O2     | 2.73                     | 0.42              |
| 35:DA:817:C:O2'    | 35:DA:839:U:OP1    | 2.37                     | 0.42              |
| 37:DC:102:GLN:O    | 37:DC:105:LEU:N    | 2.53                     | 0.42              |
| 37:DC:115:VAL:HA   | 37:DC:145:THR:CG2  | 2.48                     | 0.42              |
| 37:DC:132:LEU:HB3  | 37:DC:137:LEU:C    | 2.40                     | 0.42              |
| 38:DD:138:VAL:HA   | 38:DD:165:ILE:CG2  | 2.50                     | 0.42              |
| 39:DE:56:PRO:O     | 39:DE:57:LYS:O     | 2.36                     | 0.42              |
| 40:DF:181:LEU:O    | 40:DF:205:ARG:NH1  | 2.53                     | 0.42              |
| 40:DF:124:LEU:CD2  | 40:DF:191:ARG:HH21 | 2.32                     | 0.42              |
| 41:DG:147:ASP:C    | 41:DG:149:VAL:N    | 2.73                     | 0.42              |
| 41:DG:18:GLU:HG2   | 41:DG:175:LEU:HD13 | 2.02                     | 0.42              |
| 36:DB:42:C:C5'     | 41:DG:67:LYS:HD2   | 2.49                     | 0.42              |
| 41:DG:39:ILE:HD11  | 41:DG:92:VAL:CG2   | 2.50                     | 0.42              |
| 42:DH:103:LEU:HD12 | 42:DH:104:GLU:N    | 2.35                     | 0.42              |
| 44:DK:100:THR:CA   | 44:DK:139:VAL:HB   | 2.43                     | 0.42              |
| 44:DK:93:ARG:HB2   | 58:DZ:112:ARG:NH2  | 2.35                     | 0.42              |
| 49:DQ:75:THR:HG22  | 49:DQ:76:LYS:H     | 1.82                     | 0.42              |
| 51:DS:74:ALA:HB2   | 51:DS:101:LEU:HD22 | 2.01                     | 0.42              |
| 53:DU:37:GLU:O     | 53:DU:40:PHE:HB2   | 2.19                     | 0.42              |
| 58:DZ:9:TYR:HB3    | 58:DZ:35:ARG:NH2   | 2.33                     | 0.42              |
| 1:AA:1134:G:H2'    | 1:AA:1135:U:H5'    | 2.01                     | 0.42              |
| 1:AA:1332:A:H2'    | 1:AA:1333:A:H8     | 1.84                     | 0.42              |
| 1:AA:1423:G:P      | 47:BO:49:ARG:HH22  | 2.42                     | 0.42              |
| 1:AA:1475:G:OP1    | 35:BA:1689:A:H1'   | 2.19                     | 0.42              |
| 1:AA:271:C:H2'     | 1:AA:272:C:H6      | 1.84                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:807:A:C5      | 1:AA:808:C:C4      | 3.08                     | 0.42              |
| 2:AB:207:ALA:C     | 2:AB:209:ARG:N     | 2.71                     | 0.42              |
| 2:AB:32:ILE:O      | 2:AB:32:ILE:HG23   | 2.19                     | 0.42              |
| 3:AC:134:ILE:O     | 3:AC:135:LYS:C     | 2.58                     | 0.42              |
| 4:AD:179:GLU:C     | 4:AD:181:MET:H     | 2.23                     | 0.42              |
| 5:AE:153:LYS:H     | 8:AH:64:LYS:HZ3    | 1.68                     | 0.42              |
| 6:AF:29:ALA:O      | 6:AF:30:LEU:C      | 2.58                     | 0.42              |
| 7:AG:65:ALA:HA     | 7:AG:128:ALA:CA    | 2.49                     | 0.42              |
| 7:AG:38:LEU:O      | 7:AG:38:LEU:HD12   | 2.20                     | 0.42              |
| 9:AI:117:HIS:C     | 9:AI:118:LYS:HG3   | 2.40                     | 0.42              |
| 1:AA:1130:A:H5'    | 9:AI:18:PHE:HE1    | 1.84                     | 0.42              |
| 11:AK:79:SER:CB    | 11:AK:106:LYS:HD2  | 2.50                     | 0.42              |
| 13:AM:72:ALA:O     | 13:AM:75:ALA:N     | 2.53                     | 0.42              |
| 17:AQ:63:ARG:HG2   | 17:AQ:64:PRO:HD2   | 2.02                     | 0.42              |
| 19:AS:19:VAL:HG13  | 19:AS:44:MET:HG2   | 2.02                     | 0.42              |
| 24:AY:205:TYR:O    | 24:AY:206:LEU:C    | 2.57                     | 0.42              |
| 24:AY:580:MET:SD   | 35:BA:1913:A:N6    | 2.93                     | 0.42              |
| 25:B0:23:VAL:HG13  | 25:B0:38:VAL:HG22  | 2.02                     | 0.42              |
| 26:B1:4:VAL:HG21   | 26:B1:11:ARG:HH11  | 1.84                     | 0.42              |
| 31:B6:9:LEU:CD1    | 31:B6:26:ASN:HB2   | 2.49                     | 0.42              |
| 33:B8:25:MET:HB3   | 33:B8:26:LYS:H     | 1.69                     | 0.42              |
| 35:BA:1022:G:O2'   | 35:BA:1023:U:OP2   | 2.37                     | 0.42              |
| 35:BA:1043:C:H2'   | 35:BA:1044:G:C5'   | 2.19                     | 0.42              |
| 35:BA:1230:C:H2'   | 35:BA:1231:G:H8    | 1.84                     | 0.42              |
| 35:BA:1343:G:N3    | 35:BA:1384:A:H2    | 2.18                     | 0.42              |
| 35:BA:1493:C:C2'   | 35:BA:1493:C:O2    | 2.67                     | 0.42              |
| 35:BA:1638:C:O2'   | 35:BA:1639:U:H5'   | 2.19                     | 0.42              |
| 35:BA:1814:G:H2'   | 35:BA:1815:A:C8    | 2.54                     | 0.42              |
| 35:BA:1827:C:H2'   | 35:BA:1828:G:C5'   | 2.49                     | 0.42              |
| 35:BA:2015:A:H2'   | 35:BA:2016:U:O4'   | 2.19                     | 0.42              |
| 35:BA:2292:C:O2'   | 35:BA:2293:C:H5'   | 2.20                     | 0.42              |
| 33:B8:34:TRP:HB2   | 35:BA:2420:C:OP1   | 2.20                     | 0.42              |
| 35:BA:2428:G:C5'   | 35:BA:2429:G:OP1   | 2.67                     | 0.42              |
| 35:BA:2516:G:C6    | 35:BA:2517:C:C4    | 3.08                     | 0.42              |
| 35:BA:2840:C:H2'   | 35:BA:2841:C:C6    | 2.54                     | 0.42              |
| 35:BA:696:G:C2     | 35:BA:767:U:O2     | 2.72                     | 0.42              |
| 35:BA:750:A:C3'    | 35:BA:751:A:H5''   | 2.48                     | 0.42              |
| 35:BA:805:G:H4'    | 35:BA:806:C:OP2    | 2.20                     | 0.42              |
| 35:BA:823:G:C6     | 35:BA:824:A:C6     | 3.07                     | 0.42              |
| 35:BA:953:A:H2'    | 35:BA:954:G:H8     | 1.84                     | 0.42              |
| 37:BC:101:ILE:HG23 | 37:BC:128:LEU:HD21 | 2.01                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:BC:126:SER:C    | 37:BC:128:LEU:H    | 2.22                     | 0.42              |
| 39:BE:25:VAL:CG1   | 39:BE:181:LEU:HD12 | 2.49                     | 0.42              |
| 39:BE:78:LEU:O     | 39:BE:78:LEU:HD12  | 2.20                     | 0.42              |
| 40:BF:124:LEU:CD2  | 40:BF:191:ARG:HH21 | 2.32                     | 0.42              |
| 40:BF:31:HIS:O     | 40:BF:32:LEU:C     | 2.57                     | 0.42              |
| 36:BB:56:G:H4'     | 41:BG:27:ASN:HD21  | 1.83                     | 0.42              |
| 42:BH:70:THR:C     | 42:BH:72:ILE:N     | 2.72                     | 0.42              |
| 48:BP:46:LYS:HG2   | 48:BP:52:GLU:CG    | 2.49                     | 0.42              |
| 50:BR:56:LYS:HE2   | 50:BR:88:ARG:N     | 2.35                     | 0.42              |
| 50:BR:83:ILE:HG22  | 50:BR:83:ILE:O     | 2.19                     | 0.42              |
| 51:BS:14:VAL:CG1   | 51:BS:16:ASN:HD22  | 2.32                     | 0.42              |
| 51:BS:98:VAL:O     | 51:BS:100:ALA:N    | 2.51                     | 0.42              |
| 52:BT:74:ARG:C     | 52:BT:75:ILE:HD12  | 2.40                     | 0.42              |
| 58:BZ:29:TYR:O     | 58:BZ:30:ASN:CB    | 2.68                     | 0.42              |
| 58:BZ:71:VAL:HG11  | 58:BZ:74:VAL:HG23  | 2.01                     | 0.42              |
| 1:CA:329:A:H3'     | 1:CA:330:C:H5'     | 2.00                     | 0.42              |
| 1:CA:341:C:O2      | 1:CA:349:A:C2      | 2.73                     | 0.42              |
| 3:CC:156:ARG:NH2   | 3:CC:161:GLU:HA    | 2.34                     | 0.42              |
| 3:CC:72:LYS:HE3    | 3:CC:72:LYS:C      | 2.40                     | 0.42              |
| 5:CE:11:ILE:HG22   | 5:CE:12:LEU:N      | 2.35                     | 0.42              |
| 1:CA:15:G:H4'      | 5:CE:24:ARG:HH12   | 1.84                     | 0.42              |
| 8:CH:19:VAL:CG2    | 8:CH:21:LYS:HB2    | 2.50                     | 0.42              |
| 9:CI:117:HIS:O     | 9:CI:118:LYS:HG3   | 2.19                     | 0.42              |
| 9:CI:35:GLU:HA     | 9:CI:38:GLN:HB2    | 2.02                     | 0.42              |
| 11:CK:22:HIS:CD2   | 11:CK:22:HIS:C     | 2.92                     | 0.42              |
| 12:CL:47:LYS:NZ    | 12:CL:48:PRO:HD3   | 2.34                     | 0.42              |
| 15:CO:48:LYS:HD3   | 15:CO:48:LYS:HA    | 1.74                     | 0.42              |
| 16:CP:53:VAL:CG2   | 16:CP:54:GLU:N     | 2.82                     | 0.42              |
| 16:CP:58:TYR:CD1   | 16:CP:59:TRP:N     | 2.88                     | 0.42              |
| 20:CT:94:ALA:O     | 20:CT:95:ALA:HB3   | 2.20                     | 0.42              |
| 24:CY:170:ARG:O    | 24:CY:171:GLU:CG   | 2.68                     | 0.42              |
| 24:CY:232:LEU:N    | 24:CY:232:LEU:HD13 | 2.35                     | 0.42              |
| 24:CY:457:LEU:HD23 | 24:CY:460:GLU:OE1  | 2.18                     | 0.42              |
| 25:D0:59:LEU:HD23  | 25:D0:59:LEU:HA    | 1.85                     | 0.42              |
| 29:D4:25:TYR:N     | 29:D4:25:TYR:CD1   | 2.87                     | 0.42              |
| 30:D5:36:CYS:HG    | 30:D5:49:CYS:HB3   | 1.85                     | 0.42              |
| 31:D6:35:GLU:HB3   | 31:D6:51:GLU:N     | 2.35                     | 0.42              |
| 35:DA:1019:U:O2'   | 35:DA:1021:A:C2    | 2.71                     | 0.42              |
| 35:DA:980:A:C4     | 35:DA:1136:G:O4'   | 2.73                     | 0.42              |
| 35:DA:1301:A:HO2'  | 35:DA:1302:A:P     | 2.41                     | 0.42              |
| 35:DA:1329:U:H5'   | 35:DA:1330:C:C5    | 2.49                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:1416:G:H1'   | 35:DA:1417:C:C5    | 2.54                     | 0.42              |
| 35:DA:143:G:H2'    | 35:DA:143(A):C:C6  | 2.54                     | 0.42              |
| 35:DA:2033:A:HO2'  | 35:DA:2034:U:P     | 2.43                     | 0.42              |
| 35:DA:2103:C:H3'   | 35:DA:2104:G:H5''  | 1.99                     | 0.42              |
| 35:DA:2154:G:C2    | 35:DA:2155:G:C4    | 3.08                     | 0.42              |
| 35:DA:2246:G:H2'   | 35:DA:2247:A:C8    | 2.55                     | 0.42              |
| 35:DA:2361:A:N3    | 35:DA:2361:A:H2'   | 2.35                     | 0.42              |
| 35:DA:2665:A:H2'   | 35:DA:2666:C:O4'   | 2.20                     | 0.42              |
| 35:DA:2701:C:H2'   | 35:DA:2702:U:H2'   | 2.02                     | 0.42              |
| 35:DA:271(J):C:C2' | 35:DA:271(J):C:O2  | 2.63                     | 0.42              |
| 35:DA:285:C:H2'    | 35:DA:286:C:C5'    | 2.48                     | 0.42              |
| 35:DA:444:C:H2'    | 35:DA:445:C:C6     | 2.54                     | 0.42              |
| 35:DA:637:A:N6     | 35:DA:652:C:H4'    | 2.35                     | 0.42              |
| 35:DA:685:A:C6     | 35:DA:774:A:C2     | 3.08                     | 0.42              |
| 35:DA:784:A:HO2'   | 35:DA:785:G:H8     | 1.66                     | 0.42              |
| 35:DA:802:A:C5     | 35:DA:803:U:C4     | 3.08                     | 0.42              |
| 36:DB:40:U:O2'     | 36:DB:43:C:C5      | 2.66                     | 0.42              |
| 36:DB:96:U:H2'     | 36:DB:97:G:C8      | 2.54                     | 0.42              |
| 39:DE:145:LYS:O    | 39:DE:146:THR:C    | 2.58                     | 0.42              |
| 39:DE:183:LEU:N    | 39:DE:183:LEU:HD12 | 2.35                     | 0.42              |
| 36:DB:42:C:N4      | 41:DG:91:ARG:CZ    | 2.83                     | 0.42              |
| 42:DH:162:ILE:O    | 42:DH:162:ILE:HG13 | 2.20                     | 0.42              |
| 46:DN:3:THR:CG2    | 46:DN:4:TYR:H      | 2.29                     | 0.42              |
| 49:DQ:37:LEU:HG    | 49:DQ:129:THR:HA   | 2.02                     | 0.42              |
| 49:DQ:61:GLY:O     | 58:DZ:178:GLU:HB2  | 2.19                     | 0.42              |
| 35:DA:1278:A:C5'   | 50:DR:36:THR:HG22  | 2.48                     | 0.42              |
| 50:DR:56:LYS:C     | 50:DR:58:GLY:H     | 2.22                     | 0.42              |
| 50:DR:55:ALA:HB2   | 50:DR:79:LEU:CD1   | 2.49                     | 0.42              |
| 52:DT:108:ARG:HA   | 52:DT:111:ARG:HH11 | 1.85                     | 0.42              |
| 46:DN:38:HIS:O     | 53:DU:67:ALA:HB1   | 2.20                     | 0.42              |
| 55:DW:44:ALA:O     | 55:DW:47:VAL:N     | 2.52                     | 0.42              |
| 57:DY:13:VAL:HG22  | 57:DY:14:LEU:N     | 2.33                     | 0.42              |
| 36:DB:77:U:P       | 58:DZ:19:ARG:HH22  | 2.43                     | 0.42              |
| 1:AA:1129:C:O2'    | 1:AA:1130:A:O5'    | 2.38                     | 0.42              |
| 1:AA:151:A:C2'     | 1:AA:152:A:H5'     | 2.49                     | 0.42              |
| 1:AA:178:C:C2'     | 1:AA:179:A:H5'     | 2.49                     | 0.42              |
| 1:AA:658:G:C6      | 1:AA:749:C:N4      | 2.87                     | 0.42              |
| 2:AB:160:ASP:O     | 2:AB:161:ALA:HB2   | 2.20                     | 0.42              |
| 2:AB:235:SER:OG    | 2:AB:236:TYR:N     | 2.49                     | 0.42              |
| 2:AB:81:VAL:O      | 2:AB:82:ARG:C      | 2.58                     | 0.42              |
| 3:AC:139:GLN:O     | 3:AC:140:ARG:C     | 2.57                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:AG:64:GLN:HG2    | 7:AG:128:ALA:HB1   | 2.01                     | 0.42              |
| 8:AH:99:GLU:O      | 8:AH:100:ILE:C     | 2.58                     | 0.42              |
| 8:AH:30:ARG:CB     | 8:AH:30:ARG:NH1    | 2.83                     | 0.42              |
| 9:AI:97:LYS:N      | 9:AI:98:PRO:CD     | 2.83                     | 0.42              |
| 11:AK:21:ILE:HG13  | 11:AK:30:VAL:CG1   | 2.49                     | 0.42              |
| 12:AL:47:LYS:NZ    | 12:AL:48:PRO:HD3   | 2.35                     | 0.42              |
| 12:AL:6:THR:H      | 12:AL:9:GLN:NE2    | 2.16                     | 0.42              |
| 3:AC:29:TYR:CG     | 14:AN:36:PHE:HE1   | 2.38                     | 0.42              |
| 16:AP:1:MET:HG3    | 16:AP:65:GLN:HG3   | 2.00                     | 0.42              |
| 19:AS:11:VAL:HG23  | 19:AS:38:SER:HB2   | 2.02                     | 0.42              |
| 20:AT:30:LYS:HZ2   | 20:AT:34:LYS:CE    | 2.33                     | 0.42              |
| 20:AT:81:LYS:C     | 20:AT:83:ARG:H     | 2.23                     | 0.42              |
| 20:AT:89:ARG:HD2   | 20:AT:104:LEU:CD1  | 2.49                     | 0.42              |
| 21:AU:10:ARG:HA    | 21:AU:13:ILE:HD12  | 2.00                     | 0.42              |
| 22:AV:35:A:C2      | 23:AX:18:G:C2      | 3.08                     | 0.42              |
| 24:AY:290:LYS:HD3  | 24:AY:298:VAL:HG21 | 2.02                     | 0.42              |
| 24:AY:34:TYR:O     | 24:AY:38:ARG:HB2   | 2.19                     | 0.42              |
| 24:AY:354:ARG:O    | 24:AY:378:VAL:HG23 | 2.20                     | 0.42              |
| 24:AY:484:ARG:HD2  | 24:AY:559:PRO:HB2  | 2.02                     | 0.42              |
| 24:AY:537:GLU:H    | 24:AY:537:GLU:HG3  | 1.57                     | 0.42              |
| 27:B2:58:ALA:O     | 27:B2:61:LEU:N     | 2.53                     | 0.42              |
| 33:B8:61:LEU:HG    | 33:B8:61:LEU:H     | 1.33                     | 0.42              |
| 35:BA:1009:A:H1'   | 53:BU:59:ARG:NH1   | 2.34                     | 0.42              |
| 35:BA:1142(A):A:C6 | 35:BA:1144:G:C5    | 3.08                     | 0.42              |
| 35:BA:1461:G:H2'   | 35:BA:1462:C:C6    | 2.54                     | 0.42              |
| 35:BA:1678:G:N2    | 35:BA:1989:G:N2    | 2.57                     | 0.42              |
| 35:BA:2507:C:H2'   | 35:BA:2508:G:H8    | 1.84                     | 0.42              |
| 24:AY:21:ILE:CG1   | 35:BA:2661:G:H5''  | 2.40                     | 0.42              |
| 35:BA:2795:G:N2    | 35:BA:2796:U:H5    | 2.14                     | 0.42              |
| 35:BA:583:G:C5     | 35:BA:584:C:C5     | 3.07                     | 0.42              |
| 35:BA:598:G:H5'    | 48:BP:15:ARG:CB    | 2.43                     | 0.42              |
| 35:BA:84:A:N3      | 35:BA:85:G:H1'     | 2.34                     | 0.42              |
| 35:BA:862:G:H2'    | 35:BA:863:A:O4'    | 2.20                     | 0.42              |
| 35:BA:864:G:H21    | 35:BA:866:A:H61    | 1.67                     | 0.42              |
| 35:BA:987:G:H2'    | 35:BA:988:A:O4'    | 2.20                     | 0.42              |
| 36:BB:111:G:O2'    | 36:BB:112:U:H5'    | 2.20                     | 0.42              |
| 36:BB:58:A:H2'     | 36:BB:59:A:O4'     | 2.19                     | 0.42              |
| 37:BC:101:ILE:O    | 37:BC:101:ILE:HG22 | 2.19                     | 0.42              |
| 37:BC:127:LYS:O    | 37:BC:128:LEU:CG   | 2.67                     | 0.42              |
| 38:BD:242:ARG:HB2  | 38:BD:243:GLY:H    | 1.59                     | 0.42              |
| 35:BA:1902:C:H1'   | 38:BD:244:ARG:HG3  | 2.01                     | 0.42              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:BD:270:ILE:HD12 | 38:BD:270:ILE:N    | 2.35                     | 0.42              |
| 38:BD:34:VAL:O     | 38:BD:36:PRO:HD2   | 2.19                     | 0.42              |
| 39:BE:142:GLY:C    | 39:BE:143:ASN:ND2  | 2.73                     | 0.42              |
| 39:BE:101:ARG:CZ   | 39:BE:171:GLU:HB2  | 2.49                     | 0.42              |
| 39:BE:96:PHE:O     | 39:BE:175:VAL:HG11 | 2.20                     | 0.42              |
| 40:BF:109:GLY:HA2  | 40:BF:112:MET:HB2  | 2.01                     | 0.42              |
| 40:BF:206:ILE:CG2  | 40:BF:207:GLY:H    | 2.31                     | 0.42              |
| 41:BG:131:TYR:HE2  | 41:BG:133:LEU:CB   | 2.27                     | 0.42              |
| 42:BH:152:ARG:O    | 42:BH:153:LYS:C    | 2.56                     | 0.42              |
| 43:BJ:37:UNK:C     | 43:BJ:39:UNK:N     | 2.83                     | 0.42              |
| 44:BK:103:GLN:HA   | 44:BK:106:GLU:OE2  | 2.19                     | 0.42              |
| 46:BN:125:GLY:HA3  | 46:BN:126:PRO:O    | 2.20                     | 0.42              |
| 47:BO:69:ILE:HB    | 47:BO:77:ILE:CG2   | 2.49                     | 0.42              |
| 50:BR:10:LEU:CB    | 50:BR:17:ARG:HD3   | 2.41                     | 0.42              |
| 50:BR:76:VAL:CG1   | 50:BR:77:ARG:N     | 2.82                     | 0.42              |
| 52:BT:78:LEU:HD22  | 52:BT:78:LEU:O     | 2.19                     | 0.42              |
| 53:BU:92:ARG:CZ    | 54:BV:11:GLN:H     | 2.32                     | 0.42              |
| 54:BV:13:ARG:CG    | 54:BV:13:ARG:HH11  | 2.33                     | 0.42              |
| 54:BV:38:LEU:HD12  | 54:BV:56:SER:CA    | 2.50                     | 0.42              |
| 55:BW:44:ALA:O     | 55:BW:47:VAL:N     | 2.53                     | 0.42              |
| 57:BY:51:VAL:HG12  | 57:BY:53:PRO:CD    | 2.48                     | 0.42              |
| 58:BZ:168:GLU:OE2  | 58:BZ:168:GLU:HA   | 2.20                     | 0.42              |
| 1:CA:1009:G:C2     | 1:CA:1010:G:C8     | 3.08                     | 0.42              |
| 1:CA:1115:C:C4     | 1:CA:1116:C:C5     | 3.07                     | 0.42              |
| 1:CA:1284:C:O5'    | 1:CA:1284:C:H6     | 2.03                     | 0.42              |
| 1:CA:532:A:C2'     | 1:CA:533:A:OP1     | 2.68                     | 0.42              |
| 1:CA:784:C:H4'     | 35:DA:1837:C:OP1   | 2.20                     | 0.42              |
| 4:CD:62:GLN:O      | 4:CD:66:ARG:HD2    | 2.19                     | 0.42              |
| 5:CE:50:GLU:CG     | 5:CE:52:PRO:HD2    | 2.34                     | 0.42              |
| 6:CF:12:PRO:HG3    | 6:CF:55:ASP:OD1    | 2.19                     | 0.42              |
| 8:CH:11:THR:HA     | 8:CH:14:ARG:NH1    | 2.34                     | 0.42              |
| 8:CH:20:TYR:CE2    | 8:CH:75:ARG:HB3    | 2.55                     | 0.42              |
| 8:CH:66:GLY:O      | 8:CH:76:PRO:CB     | 2.68                     | 0.42              |
| 9:CI:125:TYR:CD2   | 9:CI:126:SER:N     | 2.87                     | 0.42              |
| 10:CJ:50:ILE:HD11  | 14:CN:41:ARG:HH11  | 1.79                     | 0.42              |
| 12:CL:98:TYR:N     | 12:CL:98:TYR:CD1   | 2.88                     | 0.42              |
| 13:CM:5:ALA:O      | 41:DG:113:ARG:NH1  | 2.53                     | 0.42              |
| 15:CO:56:LEU:HD21  | 35:DA:715:G:C2     | 2.54                     | 0.42              |
| 16:CP:1:MET:SD     | 16:CP:3:LYS:HE3    | 2.59                     | 0.42              |
| 19:CS:37:ARG:HG3   | 19:CS:37:ARG:H     | 1.43                     | 0.42              |
| 22:CV:56:C:C2      | 41:DG:83:ARG:HG2   | 2.55                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 24:CY:443:HIS:CD2   | 24:CY:450:ILE:HD11 | 2.55                     | 0.42              |
| 24:CY:512:ILE:N     | 24:CY:512:ILE:CD1  | 2.82                     | 0.42              |
| 24:CY:519:ARG:CZ    | 24:CY:677:GLN:HA   | 2.50                     | 0.42              |
| 25:D0:41:ARG:O      | 25:D0:42:GLY:O     | 2.37                     | 0.42              |
| 26:D1:83:GLU:OE2    | 26:D1:83:GLU:C     | 2.58                     | 0.42              |
| 27:D2:48:HIS:HA     | 27:D2:51:ARG:HG2   | 2.01                     | 0.42              |
| 30:D5:44:THR:HG21   | 50:DR:101:ALA:CB   | 2.28                     | 0.42              |
| 33:D8:26:LYS:HE2    | 33:D8:47:LYS:HD2   | 2.01                     | 0.42              |
| 35:DA:1666:G:O2'    | 35:DA:1667:G:H5'   | 2.20                     | 0.42              |
| 35:DA:1747(A):G:C2' | 35:DA:1748:G:C5'   | 2.76                     | 0.42              |
| 35:DA:781:A:H2      | 35:DA:1776:G:N3    | 2.18                     | 0.42              |
| 35:DA:1841:U:H2'    | 35:DA:1842:G:H8    | 1.84                     | 0.42              |
| 35:DA:2131:G:C8     | 35:DA:2133:G:N2    | 2.88                     | 0.42              |
| 35:DA:2131:G:C8     | 35:DA:2133:G:C2    | 3.08                     | 0.42              |
| 35:DA:2684:U:H2'    | 35:DA:2685:G:O4'   | 2.20                     | 0.42              |
| 35:DA:2688:U:H1'    | 35:DA:2721:A:H61   | 1.82                     | 0.42              |
| 35:DA:464:U:H2'     | 35:DA:465:G:O4'    | 2.19                     | 0.42              |
| 35:DA:605:C:C4      | 35:DA:606:U:C5     | 3.08                     | 0.42              |
| 35:DA:694:U:H2'     | 35:DA:695:G:O5'    | 2.20                     | 0.42              |
| 35:DA:877:U:C2'     | 35:DA:878:A:H5"    | 2.50                     | 0.42              |
| 37:DC:10:ALA:O      | 37:DC:13:GLU:HG2   | 2.20                     | 0.42              |
| 39:DE:101:ARG:HG3   | 39:DE:169:ASN:ND2  | 2.35                     | 0.42              |
| 39:DE:25:VAL:CG1    | 39:DE:181:LEU:HD12 | 2.48                     | 0.42              |
| 40:DF:110:LEU:HD13  | 40:DF:202:PHE:HE1  | 1.84                     | 0.42              |
| 40:DF:121:GLY:C     | 40:DF:123:LEU:H    | 2.23                     | 0.42              |
| 41:DG:117:PHE:CE1   | 41:DG:119:GLY:HA2  | 2.55                     | 0.42              |
| 41:DG:13:GLU:O      | 41:DG:14:GLU:CB    | 2.68                     | 0.42              |
| 41:DG:142:PRO:HG2   | 41:DG:143:GLU:CD   | 2.39                     | 0.42              |
| 41:DG:38:VAL:CG1    | 41:DG:93:THR:HA    | 2.49                     | 0.42              |
| 42:DH:72:ILE:O      | 42:DH:73:ALA:C     | 2.58                     | 0.42              |
| 42:DH:97:ARG:HG2    | 42:DH:97:ARG:O     | 2.20                     | 0.42              |
| 43:DJ:144:UNK:C     | 43:DJ:146:UNK:N    | 2.82                     | 0.42              |
| 44:DK:104:VAL:CG2   | 44:DK:127:ILE:HB   | 2.50                     | 0.42              |
| 46:DN:34:LEU:HD13   | 46:DN:34:LEU:HA    | 1.88                     | 0.42              |
| 47:DO:52:VAL:C      | 47:DO:53:LYS:HG3   | 2.39                     | 0.42              |
| 50:DR:79:LEU:HD22   | 50:DR:83:ILE:HB    | 2.01                     | 0.42              |
| 51:DS:67:ARG:NH2    | 51:DS:100:ALA:HB3  | 2.34                     | 0.42              |
| 54:DV:13:ARG:HH11   | 54:DV:13:ARG:CG    | 2.33                     | 0.42              |
| 55:DW:50:VAL:HG13   | 55:DW:51:LEU:N     | 2.33                     | 0.42              |
| 55:DW:62:HIS:O      | 55:DW:63:ASP:C     | 2.58                     | 0.42              |
| 56:DX:18:TYR:HA     | 56:DX:21:PHE:CE1   | 2.55                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 57:DY:80:GLY:O     | 57:DY:81:LYS:O    | 2.38                     | 0.42              |
| 58:DZ:85:HIS:ND1   | 58:DZ:86:VAL:N    | 2.67                     | 0.42              |
| 1:AA:1002:G:C8     | 1:AA:1003:G:N7    | 2.88                     | 0.42              |
| 1:AA:1403:C:O2     | 1:AA:1403:C:C2'   | 2.66                     | 0.42              |
| 1:AA:368:U:OP2     | 24:AY:353:ALA:CB  | 2.68                     | 0.42              |
| 1:AA:666:G:C2      | 1:AA:667:G:C8     | 3.08                     | 0.42              |
| 1:AA:757:U:H2'     | 1:AA:758:G:O4'    | 2.20                     | 0.42              |
| 1:AA:892:A:O2'     | 1:AA:1415:G:H4'   | 2.19                     | 0.42              |
| 1:AA:972:C:O2'     | 10:AJ:55:LYS:HB3  | 2.20                     | 0.42              |
| 2:AB:21:ARG:HA     | 2:AB:40:HIS:ND1   | 2.35                     | 0.42              |
| 3:AC:54:ARG:HG2    | 3:AC:54:ARG:NH1   | 2.34                     | 0.42              |
| 5:AE:72:GLN:NE2    | 5:AE:144:THR:HG22 | 2.33                     | 0.42              |
| 8:AH:123:GLU:O     | 8:AH:126:LYS:HB3  | 2.20                     | 0.42              |
| 9:AI:99:LEU:HD22   | 9:AI:99:LEU:N     | 2.34                     | 0.42              |
| 13:AM:34:LEU:HA    | 13:AM:34:LEU:HD23 | 1.89                     | 0.42              |
| 13:AM:37:THR:HG21  | 13:AM:56:LEU:CD2  | 2.46                     | 0.42              |
| 16:AP:57:ARG:O     | 16:AP:58:TYR:C    | 2.57                     | 0.42              |
| 19:AS:20:LEU:HA    | 19:AS:23:ASN:CB   | 2.46                     | 0.42              |
| 20:AT:84:LEU:C     | 20:AT:86:ARG:N    | 2.72                     | 0.42              |
| 22:AV:28:C:O2      | 22:AV:43:A:C2     | 2.72                     | 0.42              |
| 24:AY:250:THR:C    | 24:AY:252:ASP:H   | 2.22                     | 0.42              |
| 24:AY:357:ARG:HG3  | 24:AY:357:ARG:NH2 | 2.34                     | 0.42              |
| 24:AY:370:LYS:O    | 24:AY:371:ALA:C   | 2.58                     | 0.42              |
| 61:AY:702:FUA:H231 | 61:AY:702:FUA:C12 | 2.45                     | 0.42              |
| 32:B7:35:ARG:O     | 32:B7:38:GLY:N    | 2.48                     | 0.42              |
| 35:BA:1319:G:C2    | 35:BA:1334:G:C6   | 3.08                     | 0.42              |
| 35:BA:1348:G:C3'   | 35:BA:1349:A:H5'' | 2.49                     | 0.42              |
| 35:BA:212:G:C5'    | 35:BA:212:G:C8    | 2.98                     | 0.42              |
| 35:BA:223:A:C4     | 35:BA:422:A:C8    | 3.08                     | 0.42              |
| 35:BA:2290:G:H4'   | 35:BA:2381:C:O2'  | 2.20                     | 0.42              |
| 35:BA:2693:A:H61   | 35:BA:2716:U:H3   | 1.68                     | 0.42              |
| 35:BA:2751:G:OP1   | 35:BA:2751:G:N2   | 2.52                     | 0.42              |
| 35:BA:2837:G:H2'   | 35:BA:2838:G:H8   | 1.84                     | 0.42              |
| 35:BA:347:A:H2'    | 35:BA:348:G:C8    | 2.55                     | 0.42              |
| 35:BA:359:A:H3'    | 35:BA:360:G:C8    | 2.55                     | 0.42              |
| 35:BA:534:U:O2'    | 53:BU:49:HIS:CD2  | 2.72                     | 0.42              |
| 35:BA:545:C:H3'    | 35:BA:547:A:C5'   | 2.50                     | 0.42              |
| 35:BA:902:C:H2'    | 35:BA:903:C:H6    | 1.85                     | 0.42              |
| 36:BB:96:U:H2'     | 36:BB:97:G:C8     | 2.54                     | 0.42              |
| 37:BC:140:ASN:H    | 37:BC:145:THR:HB  | 1.85                     | 0.42              |
| 38:BD:227:ASN:O    | 38:BD:228:PRO:C   | 2.58                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 38:BD:61:LEU:HA   | 38:BD:61:LEU:HD13  | 1.76                     | 0.42              |
| 39:BE:110:GLY:HA2 | 39:BE:162:ALA:H    | 1.85                     | 0.42              |
| 39:BE:55:ASN:HA   | 39:BE:55:ASN:HD22  | 1.55                     | 0.42              |
| 39:BE:56:PRO:O    | 39:BE:57:LYS:O     | 2.38                     | 0.42              |
| 41:BG:54:GLU:C    | 41:BG:57:ALA:HB3   | 2.39                     | 0.42              |
| 41:BG:76:SER:OG   | 41:BG:83:ARG:HB3   | 2.17                     | 0.42              |
| 44:BK:6:ALA:HB1   | 44:BK:8:VAL:HG23   | 2.01                     | 0.42              |
| 45:BL:4:UNK:C     | 45:BL:6:UNK:N      | 2.83                     | 0.42              |
| 46:BN:109:LYS:HE3 | 46:BN:109:LYS:H    | 1.84                     | 0.42              |
| 46:BN:43:THR:HG22 | 46:BN:45:ASN:HD22  | 1.84                     | 0.42              |
| 47:BO:60:ALA:HA   | 47:BO:87:ILE:HD11  | 2.00                     | 0.42              |
| 47:BO:87:ILE:HG22 | 47:BO:92:GLU:C     | 2.40                     | 0.42              |
| 35:BA:624:C:N4    | 48:BP:107:LYS:HZ2  | 2.17                     | 0.42              |
| 35:BA:2467:C:O2   | 49:BQ:124:LYS:NZ   | 2.52                     | 0.42              |
| 49:BQ:136:ALA:C   | 49:BQ:138:ASP:H    | 2.22                     | 0.42              |
| 51:BS:19:LYS:C    | 51:BS:20:ARG:CZ    | 2.88                     | 0.42              |
| 51:BS:42:ASP:O    | 51:BS:43:GLU:CB    | 2.68                     | 0.42              |
| 52:BT:117:ASP:O   | 52:BT:118:ARG:C    | 2.58                     | 0.42              |
| 58:BZ:100:VAL:CG2 | 58:BZ:126:VAL:HG22 | 2.50                     | 0.42              |
| 1:CA:1258:G:C6    | 1:CA:1259:C:N4     | 2.88                     | 0.42              |
| 1:CA:1429:C:H2'   | 1:CA:1430:C:H6     | 1.84                     | 0.42              |
| 1:CA:251:G:H4'    | 1:CA:252:U:O5'     | 2.19                     | 0.42              |
| 1:CA:807:A:C5     | 1:CA:808:C:C4      | 3.08                     | 0.42              |
| 1:CA:979:C:C2'    | 1:CA:980:C:H5''    | 2.47                     | 0.42              |
| 2:CB:142:LEU:HD23 | 2:CB:142:LEU:O     | 2.19                     | 0.42              |
| 2:CB:17:PHE:O     | 2:CB:18:GLY:O      | 2.38                     | 0.42              |
| 3:CC:53:ALA:HB1   | 3:CC:114:PRO:HB2   | 2.01                     | 0.42              |
| 3:CC:22:TRP:CH2   | 3:CC:32:LEU:HB2    | 2.55                     | 0.42              |
| 4:CD:98:GLU:CB    | 4:CD:189:PRO:HG3   | 2.49                     | 0.42              |
| 4:CD:96:LEU:H     | 4:CD:96:LEU:CD2    | 2.26                     | 0.42              |
| 5:CE:92:LYS:HB3   | 5:CE:119:LEU:HB2   | 2.01                     | 0.42              |
| 8:CH:91:ARG:CG    | 8:CH:91:ARG:HH11   | 2.31                     | 0.42              |
| 9:CI:43:ALA:HA    | 9:CI:74:ILE:HG21   | 2.02                     | 0.42              |
| 9:CI:60:ASP:O     | 9:CI:61:ALA:O      | 2.37                     | 0.42              |
| 10:CJ:32:ALA:CB   | 10:CJ:78:ASN:HD21  | 2.33                     | 0.42              |
| 10:CJ:79:ARG:HD3  | 10:CJ:79:ARG:HA    | 1.67                     | 0.42              |
| 1:CA:235:C:C5'    | 17:CQ:70:ARG:HG2   | 2.44                     | 0.42              |
| 18:CR:51:LEU:HA   | 18:CR:52:PRO:HD3   | 1.81                     | 0.42              |
| 22:CV:53:G:O2'    | 22:CV:54:5MU:H5''  | 2.20                     | 0.42              |
| 24:CY:19:ALA:C    | 24:CY:121:VAL:HG11 | 2.40                     | 0.42              |
| 24:CY:33:LEU:CD1  | 24:CY:36:THR:HG21  | 2.49                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:CY:434:GLU:O    | 24:CY:434:GLU:HG2  | 2.18                     | 0.42              |
| 27:D2:30:ARG:O     | 27:D2:34:GLU:HB2   | 2.19                     | 0.42              |
| 35:DA:1204:A:H1'   | 35:DA:1206:G:N7    | 2.35                     | 0.42              |
| 35:DA:1301:A:C8    | 35:DA:1303:G:C8    | 3.08                     | 0.42              |
| 35:DA:1565:C:H2'   | 38:DD:21:PHE:CE1   | 2.55                     | 0.42              |
| 35:DA:1799:G:H22   | 35:DA:1818:U:H2'   | 1.84                     | 0.42              |
| 35:DA:2193:G:O2'   | 35:DA:2194:G:H5'   | 2.20                     | 0.42              |
| 35:DA:2295:C:H2'   | 35:DA:2296:U:C6    | 2.54                     | 0.42              |
| 35:DA:2402:C:C6    | 35:DA:2402:C:OP2   | 2.73                     | 0.42              |
| 35:DA:2597:G:H5''  | 38:DD:243:GLY:HA2  | 2.02                     | 0.42              |
| 35:DA:271(E):U:H3  | 35:DA:271(S):G:H1  | 1.68                     | 0.42              |
| 35:DA:418:G:H2'    | 35:DA:419:C:H6     | 1.85                     | 0.42              |
| 35:DA:438:G:H2'    | 35:DA:440:G:H8     | 1.85                     | 0.42              |
| 35:DA:519:U:H2'    | 35:DA:520:G:H8     | 1.85                     | 0.42              |
| 35:DA:739:G:OP2    | 35:DA:739:G:H8     | 2.02                     | 0.42              |
| 35:DA:811:U:C3'    | 35:DA:812:C:C5'    | 2.98                     | 0.42              |
| 35:DA:914:C:C2'    | 35:DA:915:C:H5'    | 2.44                     | 0.42              |
| 35:DA:953:A:H2'    | 35:DA:954:G:H8     | 1.85                     | 0.42              |
| 37:DC:132:LEU:HD22 | 37:DC:137:LEU:CB   | 2.50                     | 0.42              |
| 39:DE:116:VAL:CG2  | 39:DE:122:PHE:CG   | 3.03                     | 0.42              |
| 40:DF:39:TRP:HB2   | 40:DF:101:LEU:HD22 | 2.02                     | 0.42              |
| 40:DF:160:ASN:ND2  | 40:DF:162:LEU:HB2  | 2.31                     | 0.42              |
| 40:DF:169:ASN:OD1  | 40:DF:169:ASN:O    | 2.38                     | 0.42              |
| 42:DH:46:GLU:CG    | 42:DH:51:ARG:HB2   | 2.50                     | 0.42              |
| 46:DN:18:ALA:HB1   | 46:DN:21:LYS:HB2   | 2.02                     | 0.42              |
| 35:DA:624:C:N4     | 48:DP:107:LYS:HZ2  | 2.15                     | 0.42              |
| 48:DP:122:PRO:O    | 48:DP:123:LEU:CB   | 2.68                     | 0.42              |
| 50:DR:56:LYS:HE2   | 50:DR:88:ARG:N     | 2.35                     | 0.42              |
| 52:DT:10:VAL:C     | 52:DT:12:SER:H     | 2.22                     | 0.42              |
| 52:DT:20:PRO:O     | 52:DT:22:PHE:HD2   | 2.03                     | 0.42              |
| 54:DV:40:LEU:HD13  | 54:DV:46:VAL:H     | 1.84                     | 0.42              |
| 57:DY:54:LYS:HE2   | 57:DY:55:TYR:HE2   | 1.84                     | 0.42              |
| 57:DY:58:GLY:O     | 57:DY:59:GLY:O     | 2.38                     | 0.42              |
| 58:DZ:29:TYR:CB    | 58:DZ:34:ASN:CB    | 2.93                     | 0.42              |
| 1:AA:1054:C:O2     | 1:AA:1054:C:C2'    | 2.66                     | 0.42              |
| 1:AA:414:A:O2'     | 1:AA:415:A:H5'     | 2.20                     | 0.42              |
| 1:AA:703:G:O2'     | 1:AA:704:A:P       | 2.78                     | 0.42              |
| 1:AA:923:A:O2'     | 1:AA:924:C:H5'     | 2.20                     | 0.42              |
| 3:AC:70:VAL:HG21   | 3:AC:76:VAL:HG11   | 2.01                     | 0.42              |
| 4:AD:168:ARG:HD2   | 4:AD:168:ARG:N     | 2.33                     | 0.42              |
| 6:AF:20:ALA:O      | 6:AF:21:LEU:C      | 2.59                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:AH:100:ILE:HA    | 8:AH:101:PRO:HD3   | 1.74                     | 0.42              |
| 10:AJ:32:ALA:CB    | 10:AJ:76:ASN:HB3   | 2.50                     | 0.42              |
| 12:AL:54:LYS:O     | 12:AL:70:ILE:HG12  | 2.20                     | 0.42              |
| 12:AL:6:THR:H      | 12:AL:9:GLN:HE21   | 1.68                     | 0.42              |
| 13:AM:5:ALA:O      | 41:BG:113:ARG:NH1  | 2.53                     | 0.42              |
| 1:AA:624:C:O3'     | 16:AP:10:GLY:HA2   | 2.19                     | 0.42              |
| 22:AV:39:C:H2'     | 22:AV:40:C:C6      | 2.54                     | 0.42              |
| 1:AA:936:C:O2'     | 22:AW:35:C:H5'     | 2.20                     | 0.42              |
| 23:AX:16:A:H2'     | 23:AX:17:U:C6      | 2.55                     | 0.42              |
| 24:AY:124:GLN:HE21 | 24:AY:124:GLN:HB2  | 1.53                     | 0.42              |
| 26:B1:78:LYS:O     | 26:B1:80:LEU:N     | 2.53                     | 0.42              |
| 31:B6:41:PRO:HD3   | 31:B6:47:THR:HG22  | 2.02                     | 0.42              |
| 32:B7:25:PRO:CA    | 32:B7:28:ARG:NH2   | 2.83                     | 0.42              |
| 35:BA:1052:C:C3'   | 35:BA:1052:C:C6    | 3.02                     | 0.42              |
| 35:BA:120:U:C2'    | 35:BA:120:U:O2     | 2.60                     | 0.42              |
| 35:BA:1325:G:OP2   | 35:BA:1616:A:H2'   | 2.20                     | 0.42              |
| 35:BA:1608:A:C6    | 35:BA:1611:C:C2    | 3.07                     | 0.42              |
| 35:BA:1770:G:C2'   | 35:BA:1771:C:H5'   | 2.49                     | 0.42              |
| 35:BA:1820:U:OP1   | 35:BA:1820:U:H6    | 2.03                     | 0.42              |
| 35:BA:2033:A:O2'   | 35:BA:2034:U:P     | 2.77                     | 0.42              |
| 35:BA:2322:A:O2'   | 35:BA:2323:G:H5'   | 2.20                     | 0.42              |
| 35:BA:2825:C:H2'   | 35:BA:2826:A:O4'   | 2.20                     | 0.42              |
| 35:BA:519:U:H2'    | 35:BA:520:G:H8     | 1.84                     | 0.42              |
| 35:BA:603:A:O2'    | 35:BA:604:G:OP2    | 2.31                     | 0.42              |
| 35:BA:968:G:C6     | 35:BA:969:U:C4     | 3.08                     | 0.42              |
| 35:BA:1843:C:H5'   | 38:BD:253:GLN:NE2  | 2.34                     | 0.42              |
| 38:BD:28:GLU:CD    | 38:BD:28:GLU:N     | 2.74                     | 0.42              |
| 38:BD:73:VAL:C     | 38:BD:75:ILE:H     | 2.24                     | 0.42              |
| 39:BE:119:ARG:NH1  | 39:BE:156:MET:O    | 2.53                     | 0.42              |
| 39:BE:4:ILE:HD13   | 39:BE:28:ALA:HB1   | 2.01                     | 0.42              |
| 39:BE:79:ARG:HH11  | 39:BE:79:ARG:HG2   | 1.85                     | 0.42              |
| 40:BF:167:ALA:C    | 40:BF:170:LEU:HD23 | 2.39                     | 0.42              |
| 41:BG:103:LEU:O    | 41:BG:104:GLU:C    | 2.58                     | 0.42              |
| 41:BG:109:VAL:HG12 | 41:BG:110:ALA:N    | 2.35                     | 0.42              |
| 42:BH:46:GLU:HG2   | 42:BH:46:GLU:H     | 1.36                     | 0.42              |
| 42:BH:54:ARG:HH11  | 42:BH:54:ARG:HG2   | 1.84                     | 0.42              |
| 44:BK:27:LEU:HA    | 44:BK:30:HIS:HB2   | 2.02                     | 0.42              |
| 48:BP:89:ALA:HB1   | 48:BP:121:LYS:HD2  | 2.02                     | 0.42              |
| 50:BR:83:ILE:HA    | 50:BR:86:ARG:HD3   | 2.01                     | 0.42              |
| 51:BS:101:LEU:O    | 51:BS:102:ALA:O    | 2.38                     | 0.42              |
| 51:BS:35:ILE:HG22  | 51:BS:53:SER:HB2   | 2.02                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:BU:12:ARG:O    | 53:BU:13:LYS:C    | 2.58                     | 0.42              |
| 55:BW:31:GLU:O    | 55:BW:35:ILE:HG12 | 2.19                     | 0.42              |
| 56:BX:12:VAL:CG1  | 56:BX:27:THR:O    | 2.59                     | 0.42              |
| 58:BZ:17:ALA:O    | 58:BZ:21:ALA:HB2  | 2.19                     | 0.42              |
| 58:BZ:25:PRO:O    | 58:BZ:85:HIS:HA   | 2.19                     | 0.42              |
| 1:CA:1256:A:N6    | 1:CA:1278:U:H1'   | 2.35                     | 0.42              |
| 1:CA:1238:A:C8    | 1:CA:1303:C:H1'   | 2.55                     | 0.42              |
| 1:CA:186:C:H2'    | 1:CA:187:C:C6     | 2.55                     | 0.42              |
| 1:CA:402:G:C5     | 1:CA:403:C:C5     | 3.08                     | 0.42              |
| 1:CA:402:G:C6     | 1:CA:403:C:C4     | 3.08                     | 0.42              |
| 1:CA:631:G:H5'    | 1:CA:631:G:C8     | 2.52                     | 0.42              |
| 1:CA:663:A:C2'    | 1:CA:664:G:H5'    | 2.50                     | 0.42              |
| 2:CB:156:LYS:O    | 2:CB:157:ARG:CB   | 2.63                     | 0.42              |
| 2:CB:81:VAL:O     | 2:CB:82:ARG:C     | 2.59                     | 0.42              |
| 4:CD:50:ARG:HA    | 4:CD:51:PRO:HD3   | 1.90                     | 0.42              |
| 5:CE:101:ILE:H    | 5:CE:101:ILE:CD1  | 2.26                     | 0.42              |
| 1:CA:1130:A:H5'   | 9:CI:18:PHE:HE1   | 1.85                     | 0.42              |
| 10:CJ:34:VAL:HG13 | 10:CJ:73:ASP:O    | 2.19                     | 0.42              |
| 11:CK:93:GLN:O    | 11:CK:94:ALA:C    | 2.57                     | 0.42              |
| 16:CP:75:ARG:O    | 16:CP:77:ALA:N    | 2.51                     | 0.42              |
| 24:CY:106:VAL:CG2 | 24:CY:132:ARG:HG3 | 2.49                     | 0.42              |
| 24:CY:221:ALA:C   | 24:CY:223:PHE:H   | 2.22                     | 0.42              |
| 24:CY:370:LYS:O   | 24:CY:371:ALA:C   | 2.57                     | 0.42              |
| 26:D1:11:ARG:HB2  | 26:D1:12:PRO:HD2  | 2.01                     | 0.42              |
| 32:D7:8:ASN:HD22  | 32:D7:9:ARG:H     | 1.63                     | 0.42              |
| 33:D8:49:VAL:O    | 33:D8:53:PRO:HD3  | 2.20                     | 0.42              |
| 34:D9:18:ARG:O    | 34:D9:18:ARG:CG   | 2.57                     | 0.42              |
| 35:DA:1016:G:H1   | 35:DA:1146:C:H42  | 1.67                     | 0.42              |
| 35:DA:1090:U:O2   | 35:DA:1102:C:H1'  | 2.19                     | 0.42              |
| 35:DA:1131:G:C2   | 35:DA:1132:A:C5   | 3.08                     | 0.42              |
| 35:DA:1570:A:H2'  | 35:DA:1571:A:C8   | 2.54                     | 0.42              |
| 35:DA:1569:A:O2'  | 35:DA:1570:A:H5'  | 2.19                     | 0.42              |
| 35:DA:1654:A:OP1  | 50:DR:3:HIS:HB2   | 2.20                     | 0.42              |
| 35:DA:1722:A:C2   | 35:DA:1740:G:C8   | 3.08                     | 0.42              |
| 35:DA:1891:G:O5'  | 35:DA:1891:G:H8   | 2.02                     | 0.42              |
| 35:DA:190:A:H3'   | 35:DA:204:A:H61   | 1.85                     | 0.42              |
| 35:DA:2184:G:H2'  | 35:DA:2185:C:C6   | 2.54                     | 0.42              |
| 35:DA:239:U:H1'   | 35:DA:259:G:N2    | 2.34                     | 0.42              |
| 35:DA:2713:A:H4'  | 35:DA:2713:A:OP2  | 2.19                     | 0.42              |
| 35:DA:347:A:H2'   | 35:DA:348:G:C8    | 2.55                     | 0.42              |
| 35:DA:360:G:O2'   | 35:DA:361:G:H5'   | 2.19                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:DA:700:G:H2'   | 35:DA:701:G:H8     | 1.84                     | 0.42              |
| 35:DA:724:U:O2'   | 35:DA:725:G:H5'    | 2.20                     | 0.42              |
| 35:DA:977:G:H2'   | 35:DA:978:G:H8     | 1.84                     | 0.42              |
| 37:DC:149:ASN:C   | 37:DC:149:ASN:ND2  | 2.73                     | 0.42              |
| 37:DC:7:ARG:O     | 37:DC:11:LEU:HG    | 2.19                     | 0.42              |
| 40:DF:170:LEU:N   | 40:DF:170:LEU:CD2  | 2.83                     | 0.42              |
| 40:DF:22:ALA:C    | 40:DF:24:LEU:N     | 2.72                     | 0.42              |
| 40:DF:81:PRO:C    | 40:DF:83:PHE:N     | 2.73                     | 0.42              |
| 41:DG:5:VAL:H     | 41:DG:8:LYS:HB3    | 1.84                     | 0.42              |
| 43:DJ:153:UNK:C   | 43:DJ:155:UNK:N    | 2.82                     | 0.42              |
| 46:DN:133:GLN:CG  | 46:DN:135:PRO:HD3  | 2.38                     | 0.42              |
| 35:DA:832:G:OP1   | 48:DP:40:SER:HB3   | 2.20                     | 0.42              |
| 52:DT:33:LYS:NZ   | 52:DT:43:GLN:NE2   | 2.67                     | 0.42              |
| 53:DU:29:SER:OG   | 53:DU:30:LYS:HE2   | 2.20                     | 0.42              |
| 54:DV:46:VAL:HG22 | 54:DV:47:VAL:N     | 2.25                     | 0.42              |
| 57:DY:77:PRO:O    | 57:DY:78:ALA:CB    | 2.68                     | 0.42              |
| 57:DY:7:VAL:HG21  | 57:DY:8:LYS:HZ1    | 1.85                     | 0.42              |
| 1:AA:1245:A:C2    | 1:AA:1293:G:C2     | 3.08                     | 0.41              |
| 1:AA:1349:A:OP1   | 9:AI:120:ARG:HB2   | 2.20                     | 0.41              |
| 1:AA:1430:C:C2    | 1:AA:1471:G:C2     | 3.08                     | 0.41              |
| 1:AA:1479:C:H2'   | 1:AA:1480:G:C8     | 2.52                     | 0.41              |
| 1:AA:189(B):C:C2  | 1:AA:189(J):G:C2   | 3.08                     | 0.41              |
| 1:AA:688:G:H2'    | 1:AA:689:C:C6      | 2.54                     | 0.41              |
| 1:AA:724:G:O2'    | 1:AA:725:G:H5'     | 2.20                     | 0.41              |
| 1:AA:793:U:C3'    | 1:AA:794:A:C5'     | 2.92                     | 0.41              |
| 2:AB:178:ARG:CG   | 2:AB:178:ARG:NH1   | 2.80                     | 0.41              |
| 2:AB:25:ASN:O     | 2:AB:27:LYS:N      | 2.53                     | 0.41              |
| 2:AB:60:ASP:O     | 2:AB:64:ARG:CZ     | 2.68                     | 0.41              |
| 2:AB:82:ARG:NH1   | 2:AB:82:ARG:HG3    | 2.35                     | 0.41              |
| 3:AC:78:GLY:CA    | 3:AC:83:ARG:HB3    | 2.49                     | 0.41              |
| 4:AD:159:ARG:O    | 4:AD:160:GLN:C     | 2.58                     | 0.41              |
| 4:AD:91:SER:O     | 4:AD:92:VAL:C      | 2.57                     | 0.41              |
| 7:AG:79:ARG:O     | 7:AG:80:VAL:HG13   | 2.19                     | 0.41              |
| 10:AJ:32:ALA:HB1  | 10:AJ:76:ASN:HB3   | 2.02                     | 0.41              |
| 11:AK:31:THR:O    | 11:AK:31:THR:CG2   | 2.68                     | 0.41              |
| 12:AL:117:ARG:O   | 12:AL:119:LYS:O    | 2.36                     | 0.41              |
| 10:AJ:50:ILE:CD1  | 14:AN:41:ARG:HD3   | 2.50                     | 0.41              |
| 17:AQ:59:ILE:HD13 | 17:AQ:59:ILE:HA    | 1.79                     | 0.41              |
| 20:AT:81:LYS:C    | 20:AT:83:ARG:N     | 2.73                     | 0.41              |
| 22:AV:4:G:O2'     | 22:AV:5:G:C8       | 2.69                     | 0.41              |
| 24:AY:134:ALA:HB3 | 24:AY:258:VAL:HG22 | 2.02                     | 0.41              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:AY:348:ARG:HG2  | 24:AY:382:GLU:HG3  | 2.01                     | 0.41              |
| 24:AY:443:HIS:HA   | 24:AY:444:PRO:HD2  | 1.92                     | 0.41              |
| 24:AY:553:GLY:H    | 24:AY:557:GLY:C    | 2.23                     | 0.41              |
| 24:AY:9:LEU:HA     | 24:AY:12:LEU:HD23  | 2.02                     | 0.41              |
| 26:B1:56:GLN:CA    | 26:B1:56:GLN:NE2   | 2.82                     | 0.41              |
| 32:B7:46:VAL:HG12  | 32:B7:47:ARG:H     | 1.83                     | 0.41              |
| 34:B9:19:ARG:O     | 34:B9:20:HIS:HB2   | 2.20                     | 0.41              |
| 35:BA:1227:G:O2'   | 35:BA:1228:G:H5'   | 2.20                     | 0.41              |
| 35:BA:1453:U:H2'   | 35:BA:1455:G:C8    | 2.55                     | 0.41              |
| 35:BA:2468:G:N2    | 35:BA:2481:G:O2'   | 2.54                     | 0.41              |
| 35:BA:2617:C:H2'   | 35:BA:2618:G:H5'   | 2.01                     | 0.41              |
| 35:BA:2740:A:H2'   | 35:BA:2741:A:C8    | 2.55                     | 0.41              |
| 35:BA:27:G:H2'     | 35:BA:28:A:OP2     | 2.19                     | 0.41              |
| 35:BA:360:G:O2'    | 35:BA:361:G:H5'    | 2.19                     | 0.41              |
| 35:BA:430:G:H2'    | 35:BA:431:U:H5'    | 2.01                     | 0.41              |
| 35:BA:436:C:H2'    | 35:BA:437:G:H8     | 1.85                     | 0.41              |
| 35:BA:444:C:H2'    | 35:BA:445:C:H6     | 1.85                     | 0.41              |
| 35:BA:482:A:N6     | 35:BA:506:G:C8     | 2.88                     | 0.41              |
| 35:BA:528:A:N1     | 35:BA:2042:A:H2'   | 2.35                     | 0.41              |
| 35:BA:643:A:H2'    | 35:BA:644:A:O4'    | 2.20                     | 0.41              |
| 35:BA:826:U:H2'    | 35:BA:828:U:O4'    | 2.19                     | 0.41              |
| 38:BD:8:PRO:C      | 38:BD:10:THR:H     | 2.23                     | 0.41              |
| 38:BD:239:ARG:NH2  | 38:BD:239:ARG:HG2  | 2.34                     | 0.41              |
| 38:BD:34:VAL:CG2   | 38:BD:35:LYS:H     | 2.04                     | 0.41              |
| 35:BA:2820:A:H8    | 39:BE:191:PRO:HB3  | 1.85                     | 0.41              |
| 40:BF:28:ILE:N     | 40:BF:28:ILE:CD1   | 2.80                     | 0.41              |
| 41:BG:86:MET:N     | 41:BG:87:PRO:CD    | 2.75                     | 0.41              |
| 42:BH:162:ILE:O    | 42:BH:162:ILE:HG13 | 2.20                     | 0.41              |
| 43:BJ:72:UNK:C     | 43:BJ:74:UNK:N     | 2.82                     | 0.41              |
| 48:BP:16:ARG:NH2   | 48:BP:18:ARG:HG3   | 2.35                     | 0.41              |
| 48:BP:47:ASP:OD1   | 48:BP:48:PRO:O     | 2.38                     | 0.41              |
| 50:BR:56:LYS:C     | 50:BR:58:GLY:H     | 2.23                     | 0.41              |
| 51:BS:17:ARG:C     | 51:BS:19:LYS:H     | 2.23                     | 0.41              |
| 52:BT:12:SER:O     | 52:BT:15:VAL:HG13  | 2.19                     | 0.41              |
| 52:BT:85:LYS:NZ    | 52:BT:85:LYS:CB    | 2.71                     | 0.41              |
| 55:BW:68:ARG:HA    | 55:BW:110:LYS:CG   | 2.48                     | 0.41              |
| 57:BY:52:SER:O     | 57:BY:53:PRO:C     | 2.59                     | 0.41              |
| 1:CA:1162:C:C2     | 1:CA:1175:G:N2     | 2.88                     | 0.41              |
| 1:CA:1202:G:H2'    | 1:CA:1203:C:H5'    | 2.01                     | 0.41              |
| 1:CA:1329:A:H5''   | 13:CM:26:GLY:N     | 2.35                     | 0.41              |
| 1:CA:1442(A):G:H2' | 52:DT:118:ARG:HH11 | 1.85                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:253:U:H2'    | 1:CA:254:G:H8      | 1.84                     | 0.41              |
| 1:CA:333:G:O2'    | 1:CA:334:C:H5'     | 2.20                     | 0.41              |
| 1:CA:78:G:C2      | 1:CA:79:G:H1'      | 2.55                     | 0.41              |
| 1:CA:757:U:O2'    | 1:CA:879:C:H1'     | 2.19                     | 0.41              |
| 2:CB:166:ASP:HA   | 2:CB:167:PRO:HD2   | 1.93                     | 0.41              |
| 4:CD:105:VAL:HG13 | 4:CD:110:PHE:HB2   | 2.02                     | 0.41              |
| 4:CD:170:VAL:O    | 4:CD:171:GLY:C     | 2.56                     | 0.41              |
| 1:CA:8:A:C6       | 4:CD:209:ARG:HB2   | 2.55                     | 0.41              |
| 4:CD:43:HIS:HB3   | 4:CD:46:LYS:HD3    | 2.02                     | 0.41              |
| 4:CD:58:LEU:CD2   | 4:CD:58:LEU:C      | 2.88                     | 0.41              |
| 5:CE:33:VAL:CG1   | 5:CE:34:VAL:N      | 2.81                     | 0.41              |
| 12:CL:54:LYS:HB3  | 12:CL:70:ILE:HG13  | 2.02                     | 0.41              |
| 13:CM:81:LEU:O    | 13:CM:89:GLY:HA3   | 2.20                     | 0.41              |
| 13:CM:89:GLY:O    | 13:CM:90:LEU:O     | 2.38                     | 0.41              |
| 15:CO:9:GLN:O     | 15:CO:11:VAL:N     | 2.53                     | 0.41              |
| 17:CQ:88:TYR:O    | 17:CQ:89:LEU:C     | 2.58                     | 0.41              |
| 6:CF:97:PHE:N     | 18:CR:30:ASP:OD1   | 2.52                     | 0.41              |
| 18:CR:45:SER:OG   | 18:CR:46:GLU:N     | 2.51                     | 0.41              |
| 19:CS:25:LYS:O    | 19:CS:26:GLY:C     | 2.59                     | 0.41              |
| 1:CA:1318:A:C1'   | 19:CS:37:ARG:HH21  | 2.06                     | 0.41              |
| 19:CS:11:VAL:HG23 | 19:CS:38:SER:HB2   | 2.02                     | 0.41              |
| 19:CS:50:ALA:O    | 19:CS:51:VAL:C     | 2.58                     | 0.41              |
| 19:CS:64:GLU:HG2  | 29:D4:48:ARG:HH22  | 1.82                     | 0.41              |
| 24:CY:126:GLU:O   | 24:CY:128:TYR:N    | 2.53                     | 0.41              |
| 24:CY:204:GLU:O   | 24:CY:205:TYR:C    | 2.57                     | 0.41              |
| 24:CY:170:ARG:NH2 | 24:CY:205:TYR:HE1  | 2.17                     | 0.41              |
| 24:CY:407:PRO:O   | 24:CY:408:VAL:HG13 | 2.20                     | 0.41              |
| 22:CV:36:U:OP1    | 24:CY:573:HIS:HE1  | 2.03                     | 0.41              |
| 24:CY:573:HIS:HD2 | 24:CY:575:VAL:H    | 1.68                     | 0.41              |
| 27:D2:21:LEU:CD1  | 27:D2:64:LEU:HG    | 2.50                     | 0.41              |
| 27:D2:35:LEU:HD11 | 27:D2:49:LYS:HB3   | 2.00                     | 0.41              |
| 29:D4:43:TYR:HD2  | 29:D4:44:THR:HG23  | 1.85                     | 0.41              |
| 31:D6:9:LEU:CD1   | 31:D6:28:ARG:HG2   | 2.50                     | 0.41              |
| 31:D6:9:LEU:HD21  | 31:D6:26:ASN:HD22  | 1.84                     | 0.41              |
| 35:DA:1196:C:O4'  | 35:DA:1226:A:C2    | 2.73                     | 0.41              |
| 35:DA:1854:A:H2'  | 35:DA:1855:G:O4'   | 2.20                     | 0.41              |
| 35:DA:562:U:C4    | 35:DA:2036:C:H1'   | 2.55                     | 0.41              |
| 35:DA:294:A:N6    | 35:DA:345:A:H1'    | 2.35                     | 0.41              |
| 35:DA:272(I):U:C5 | 35:DA:363(A):A:C2  | 3.07                     | 0.41              |
| 35:DA:476:G:H4'   | 35:DA:502:A:N1     | 2.35                     | 0.41              |
| 35:DA:602:G:C2    | 35:DA:656:G:C6     | 3.07                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:DA:782:A:N1    | 38:DD:226:MET:HE3 | 2.34                     | 0.41              |
| 29:D4:3:GLU:HG2   | 36:DB:40:U:C4     | 2.55                     | 0.41              |
| 37:DC:100:ILE:O   | 37:DC:102:GLN:N   | 2.53                     | 0.41              |
| 37:DC:16:ASP:O    | 37:DC:18:ASN:N    | 2.52                     | 0.41              |
| 39:DE:101:ARG:HA  | 39:DE:101:ARG:HD3 | 1.67                     | 0.41              |
| 39:DE:138:PRO:HG2 | 39:DE:139:GLY:N   | 2.35                     | 0.41              |
| 40:DF:116:ASP:OD1 | 40:DF:119:ARG:NH2 | 2.47                     | 0.41              |
| 40:DF:152:GLU:HB3 | 40:DF:190:GLU:HB2 | 2.01                     | 0.41              |
| 41:DG:34:LEU:HB2  | 41:DG:99:MET:HE1  | 2.02                     | 0.41              |
| 41:DG:46:ALA:C    | 41:DG:51:ARG:HG3  | 2.41                     | 0.41              |
| 44:DK:34:ILE:H    | 44:DK:34:ILE:HG12 | 1.59                     | 0.41              |
| 46:DN:130:HIS:O   | 46:DN:130:HIS:CG  | 2.72                     | 0.41              |
| 47:DO:17:ARG:HH21 | 47:DO:47:ILE:HD11 | 1.83                     | 0.41              |
| 50:DR:76:VAL:CG1  | 50:DR:77:ARG:N    | 2.83                     | 0.41              |
| 51:DS:19:LYS:C    | 51:DS:20:ARG:CZ   | 2.89                     | 0.41              |
| 51:DS:98:VAL:HG12 | 51:DS:100:ALA:CB  | 2.50                     | 0.41              |
| 52:DT:35:LYS:HZ1  | 52:DT:41:ARG:NH1  | 2.17                     | 0.41              |
| 53:DU:8:VAL:O     | 53:DU:9:VAL:C     | 2.57                     | 0.41              |
| 35:DA:748:G:C8    | 55:DW:89:ALA:HB1  | 2.55                     | 0.41              |
| 56:DX:53:LYS:HB3  | 56:DX:82:GLN:HB3  | 2.02                     | 0.41              |
| 56:DX:47:PHE:CD2  | 56:DX:89:ILE:HG21 | 2.55                     | 0.41              |
| 58:DZ:72:ARG:HG3  | 58:DZ:72:ARG:NH1  | 2.34                     | 0.41              |
| 1:AA:1001(A):G:H8 | 1:AA:1002:G:C8    | 2.38                     | 0.41              |
| 1:AA:108:G:N2     | 1:AA:109:A:H2     | 2.18                     | 0.41              |
| 1:AA:1100:C:C2'   | 1:AA:1101:A:H5''  | 2.48                     | 0.41              |
| 1:AA:123:C:OP1    | 1:AA:311:C:O2'    | 2.38                     | 0.41              |
| 1:AA:1305:G:H22   | 1:AA:1331:G:C2'   | 2.30                     | 0.41              |
| 1:AA:1310:G:C2    | 1:AA:1328:C:N3    | 2.88                     | 0.41              |
| 1:AA:1342:C:H1'   | 9:AI:124:GLN:CG   | 2.49                     | 0.41              |
| 1:AA:573:A:C2     | 1:AA:574:A:C2     | 3.08                     | 0.41              |
| 1:AA:625:G:H4'    | 16:AP:16:HIS:HD2  | 1.82                     | 0.41              |
| 2:AB:23:ARG:HA    | 2:AB:23:ARG:HD2   | 1.88                     | 0.41              |
| 2:AB:96:ARG:N     | 2:AB:96:ARG:CD    | 2.82                     | 0.41              |
| 3:AC:120:VAL:O    | 3:AC:121:ALA:C    | 2.57                     | 0.41              |
| 3:AC:50:ALA:HA    | 3:AC:72:LYS:HB3   | 2.02                     | 0.41              |
| 3:AC:83:ARG:O     | 3:AC:85:ARG:N     | 2.53                     | 0.41              |
| 6:AF:15:ASP:O     | 6:AF:17:SER:N     | 2.52                     | 0.41              |
| 8:AH:53:VAL:HB    | 8:AH:58:TYR:CE1   | 2.55                     | 0.41              |
| 11:AK:23:ALA:O    | 11:AK:86:GLY:HA3  | 2.19                     | 0.41              |
| 11:AK:66:LEU:O    | 11:AK:67:ASP:C    | 2.58                     | 0.41              |
| 12:AL:57:LYS:CG   | 12:AL:67:THR:HG22 | 2.47                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:AM:16:ASP:N     | 13:AM:16:ASP:OD2   | 2.52                     | 0.41              |
| 15:AO:17:ARG:HD3   | 15:AO:26:GLU:CG    | 2.48                     | 0.41              |
| 15:AO:24:SER:O     | 15:AO:25:THR:C     | 2.57                     | 0.41              |
| 15:AO:39:LEU:HD22  | 15:AO:43:LEU:HG    | 2.01                     | 0.41              |
| 15:AO:67:LEU:HA    | 15:AO:67:LEU:HD23  | 1.88                     | 0.41              |
| 16:AP:9:PHE:HE2    | 16:AP:18:ARG:CD    | 2.32                     | 0.41              |
| 20:AT:54:LYS:HA    | 20:AT:57:ARG:NH2   | 2.35                     | 0.41              |
| 20:AT:58:LYS:O     | 20:AT:59:ALA:C     | 2.57                     | 0.41              |
| 22:AW:25:U:H2'     | 22:AW:26:C:H6      | 1.82                     | 0.41              |
| 24:AY:145:ASP:HB3  | 24:AY:148:LEU:HB2  | 2.02                     | 0.41              |
| 24:AY:21:ILE:HG21  | 24:AY:88:VAL:CG1   | 2.44                     | 0.41              |
| 24:AY:229:LEU:C    | 24:AY:231:TYR:N    | 2.73                     | 0.41              |
| 24:AY:484:ARG:CD   | 24:AY:559:PRO:HB2  | 2.50                     | 0.41              |
| 25:B0:50:ASN:CA    | 25:B0:62:LEU:HD12  | 2.41                     | 0.41              |
| 26:B1:71:TYR:N     | 26:B1:71:TYR:CD1   | 2.88                     | 0.41              |
| 30:B5:2:ALA:HB2    | 35:BA:2015:A:O4'   | 2.20                     | 0.41              |
| 30:B5:40:LYS:NZ    | 30:B5:46:CYS:N     | 2.59                     | 0.41              |
| 35:BA:104:U:C6     | 35:BA:105:C:C6     | 3.08                     | 0.41              |
| 35:BA:1022:G:H22   | 35:BA:1142(A):A:H2 | 1.65                     | 0.41              |
| 35:BA:1147:C:H2'   | 35:BA:1148:A:H8    | 1.85                     | 0.41              |
| 35:BA:1185:C:H5'   | 35:BA:1186:G:OP1   | 2.20                     | 0.41              |
| 35:BA:1640:C:H2'   | 35:BA:1641:A:O4'   | 2.20                     | 0.41              |
| 35:BA:1877:A:H5'   | 35:BA:1878:G:OP2   | 2.20                     | 0.41              |
| 35:BA:1943:U:C2'   | 35:BA:1943:U:O2    | 2.67                     | 0.41              |
| 35:BA:2003:G:C6    | 35:BA:2004:G:C5    | 3.08                     | 0.41              |
| 35:BA:2093:G:C6    | 35:BA:2225:A:C8    | 3.08                     | 0.41              |
| 30:B5:29:THR:HG21  | 35:BA:2814:C:O2'   | 2.19                     | 0.41              |
| 35:BA:452:G:N3     | 35:BA:457:A:H2     | 2.18                     | 0.41              |
| 35:BA:737:C:O2'    | 35:BA:738:G:H5'    | 2.20                     | 0.41              |
| 38:BD:165:ILE:HD13 | 38:BD:175:LEU:CD2  | 2.49                     | 0.41              |
| 38:BD:73:VAL:O     | 38:BD:75:ILE:N     | 2.54                     | 0.41              |
| 40:BF:134:GLY:HA3  | 40:BF:165:ARG:NH1  | 2.35                     | 0.41              |
| 40:BF:32:LEU:C     | 40:BF:32:LEU:CD2   | 2.88                     | 0.41              |
| 40:BF:89:VAL:O     | 40:BF:91:GLY:N     | 2.49                     | 0.41              |
| 46:BN:3:THR:CG2    | 46:BN:4:TYR:N      | 2.79                     | 0.41              |
| 46:BN:65:LYS:HB3   | 46:BN:65:LYS:NZ    | 2.30                     | 0.41              |
| 47:BO:13:ASN:ND2   | 47:BO:97:ARG:HB2   | 2.36                     | 0.41              |
| 48:BP:110:TYR:O    | 48:BP:111:ARG:O    | 2.38                     | 0.41              |
| 49:BQ:55:VAL:HG23  | 58:BZ:178:GLU:HG2  | 2.01                     | 0.41              |
| 50:BR:88:ARG:HD2   | 50:BR:88:ARG:O     | 2.20                     | 0.41              |
| 51:BS:49:VAL:CG1   | 51:BS:50:SER:H     | 2.23                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:BS:67:ARG:O     | 51:BS:70:GLY:N     | 2.53                     | 0.41              |
| 52:BT:126:ALA:C    | 52:BT:128:GLU:N    | 2.73                     | 0.41              |
| 52:BT:55:ASN:O     | 52:BT:55:ASN:CG    | 2.59                     | 0.41              |
| 53:BU:102:GLU:HG3  | 54:BV:2:PHE:CE1    | 2.55                     | 0.41              |
| 55:BW:14:PRO:CG    | 55:BW:78:GLU:HB2   | 2.49                     | 0.41              |
| 58:BZ:100:VAL:HG21 | 58:BZ:126:VAL:HG21 | 2.01                     | 0.41              |
| 58:BZ:78:LYS:N     | 58:BZ:78:LYS:HD3   | 2.35                     | 0.41              |
| 1:CA:1239:A:H62    | 1:CA:1299:A:H62    | 1.68                     | 0.41              |
| 1:CA:1300:G:O2'    | 1:CA:1301:U:OP2    | 2.38                     | 0.41              |
| 1:CA:1305:G:H5''   | 21:CU:4:GLY:C      | 2.40                     | 0.41              |
| 1:CA:282:A:H3'     | 1:CA:283:C:C6      | 2.55                     | 0.41              |
| 1:CA:59:A:H3'      | 1:CA:331:G:N2      | 2.35                     | 0.41              |
| 1:CA:520:A:N1      | 1:CA:536:C:H1'     | 2.35                     | 0.41              |
| 3:CC:80:GLY:HA3    | 3:CC:82:GLU:OE1    | 2.20                     | 0.41              |
| 4:CD:126:ILE:CD1   | 4:CD:126:ILE:N     | 2.83                     | 0.41              |
| 4:CD:60:GLU:OE2    | 4:CD:198:VAL:HA    | 2.20                     | 0.41              |
| 4:CD:68:TYR:O      | 4:CD:69:GLY:C      | 2.58                     | 0.41              |
| 5:CE:50:GLU:HB3    | 5:CE:53:LEU:HG     | 2.02                     | 0.41              |
| 7:CG:143:ARG:O     | 7:CG:145:ALA:O     | 2.38                     | 0.41              |
| 7:CG:61:VAL:O      | 7:CG:62:PHE:C      | 2.58                     | 0.41              |
| 10:CJ:29:ARG:HH11  | 10:CJ:29:ARG:CG    | 2.31                     | 0.41              |
| 12:CL:110:VAL:HG21 | 12:CL:120:TYR:CD2  | 2.54                     | 0.41              |
| 19:CS:20:LEU:HA    | 19:CS:23:ASN:CB    | 2.47                     | 0.41              |
| 22:CV:24:U:H2'     | 22:CV:25:C:H6      | 1.84                     | 0.41              |
| 1:CA:368:U:P       | 24:CY:351:ARG:HH11 | 2.43                     | 0.41              |
| 24:CY:408:VAL:HG22 | 24:CY:454:MET:HA   | 2.02                     | 0.41              |
| 24:CY:590:ILE:HA   | 24:CY:590:ILE:HD13 | 1.85                     | 0.41              |
| 24:CY:603:GLU:C    | 24:CY:676:TYR:HD1  | 2.23                     | 0.41              |
| 24:CY:637:ARG:HG3  | 24:CY:637:ARG:NH1  | 2.32                     | 0.41              |
| 24:CY:25:LYS:NZ    | 62:CY:703:GDP:PB   | 2.93                     | 0.41              |
| 24:CY:88:VAL:O     | 24:CY:90:PHE:HD1   | 2.03                     | 0.41              |
| 31:D6:15:GLU:N     | 31:D6:49:HIS:CD2   | 2.88                     | 0.41              |
| 33:D8:36:LYS:O     | 33:D8:37:SER:O     | 2.38                     | 0.41              |
| 33:D8:59:LYS:HD3   | 48:DP:50:ARG:HB3   | 2.02                     | 0.41              |
| 35:DA:1024:G:C8    | 35:DA:1025:G:H2'   | 2.55                     | 0.41              |
| 35:DA:1159:U:H5''  | 35:DA:1159:U:H6    | 1.85                     | 0.41              |
| 35:DA:1485:G:H8    | 35:DA:1485:G:H5'   | 1.85                     | 0.41              |
| 35:DA:1830:C:O5'   | 35:DA:1830:C:H6    | 2.03                     | 0.41              |
| 35:DA:1948:G:O2'   | 35:DA:1949:G:H5'   | 2.19                     | 0.41              |
| 35:DA:1956:U:H2'   | 35:DA:1957:C:H5'   | 2.02                     | 0.41              |
| 35:DA:1669:A:C2    | 35:DA:1994:C:H1'   | 2.55                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:DA:2031:A:N3   | 35:DA:2455:G:O2'   | 2.47                     | 0.41              |
| 35:DA:2154:G:H2'  | 35:DA:2155:G:H8    | 1.85                     | 0.41              |
| 35:DA:2167:U:H2'  | 35:DA:2168:G:O4'   | 2.20                     | 0.41              |
| 35:DA:2384:G:H2'  | 35:DA:2386:C:OP1   | 2.20                     | 0.41              |
| 35:DA:2464:C:O2'  | 35:DA:2465:C:P     | 2.78                     | 0.41              |
| 35:DA:2511:U:H4'  | 39:DE:123:ALA:HB3  | 2.02                     | 0.41              |
| 35:DA:2616:C:H2'  | 35:DA:2616:C:O2    | 2.21                     | 0.41              |
| 35:DA:2832:U:H1'  | 35:DA:2834:G:C4    | 2.55                     | 0.41              |
| 35:DA:438:G:H2'   | 35:DA:440:G:C8     | 2.56                     | 0.41              |
| 35:DA:566:U:O4    | 54:DV:78:LYS:HE3   | 2.19                     | 0.41              |
| 35:DA:657:U:H2'   | 35:DA:658:C:C5     | 2.54                     | 0.41              |
| 36:DB:69:G:C2     | 36:DB:70:C:C2      | 3.08                     | 0.41              |
| 37:DC:11:LEU:C    | 37:DC:13:GLU:H     | 2.22                     | 0.41              |
| 38:DD:148:GLU:CB  | 38:DD:151:LYS:HG3  | 2.49                     | 0.41              |
| 39:DE:34:VAL:HG13 | 39:DE:34:VAL:O     | 2.21                     | 0.41              |
| 42:DH:19:VAL:CG1  | 42:DH:20:ALA:N     | 2.83                     | 0.41              |
| 42:DH:50:VAL:CG1  | 42:DH:51:ARG:N     | 2.83                     | 0.41              |
| 47:DO:103:ALA:O   | 47:DO:106:LEU:HG   | 2.19                     | 0.41              |
| 48:DP:91:PHE:HZ   | 48:DP:100:LEU:CD1  | 2.31                     | 0.41              |
| 49:DQ:27:VAL:O    | 49:DQ:28:ALA:CB    | 2.67                     | 0.41              |
| 50:DR:48:VAL:O    | 50:DR:51:LEU:N     | 2.53                     | 0.41              |
| 53:DU:107:ALA:HA  | 53:DU:110:VAL:HG21 | 2.02                     | 0.41              |
| 53:DU:92:ARG:NH1  | 54:DV:11:GLN:CG    | 2.83                     | 0.41              |
| 55:DW:26:GLY:HA2  | 55:DW:71:VAL:O     | 2.19                     | 0.41              |
| 58:DZ:171:ILE:C   | 58:DZ:171:ILE:HD12 | 2.40                     | 0.41              |
| 58:DZ:17:ALA:HA   | 58:DZ:20:ARG:CD    | 2.50                     | 0.41              |
| 58:DZ:63:ASP:HB2  | 58:DZ:65:GLN:HG3   | 2.02                     | 0.41              |
| 58:DZ:82:ARG:HG2  | 58:DZ:82:ARG:HH11  | 1.84                     | 0.41              |
| 1:AA:1026:G:H3'   | 1:AA:1027:C:H5'    | 2.01                     | 0.41              |
| 1:AA:1055:A:H8    | 1:AA:1055:A:O5'    | 2.04                     | 0.41              |
| 1:AA:1329:A:H5''  | 13:AM:26:GLY:N     | 2.36                     | 0.41              |
| 1:AA:142:G:N3     | 1:AA:196:A:H2      | 2.18                     | 0.41              |
| 1:AA:674:G:O4'    | 18:AR:81:PHE:CE1   | 2.74                     | 0.41              |
| 1:AA:748:C:O2'    | 1:AA:749:C:H6      | 2.03                     | 0.41              |
| 2:AB:187:LEU:HD21 | 2:AB:214:ILE:HG13  | 2.02                     | 0.41              |
| 3:AC:72:LYS:HE3   | 3:AC:72:LYS:C      | 2.40                     | 0.41              |
| 8:AH:36:LEU:O     | 8:AH:37:ARG:C      | 2.59                     | 0.41              |
| 9:AI:97:LYS:O     | 9:AI:98:PRO:C      | 2.59                     | 0.41              |
| 10:AJ:50:ILE:HD11 | 14:AN:41:ARG:HH11  | 1.80                     | 0.41              |
| 12:AL:44:THR:HA   | 12:AL:45:PRO:HD3   | 1.82                     | 0.41              |
| 12:AL:46:LYS:NZ   | 12:AL:94:PRO:HG3   | 2.34                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 13:AM:49:THR:HG22  | 13:AM:51:ALA:N      | 2.16                     | 0.41              |
| 15:AO:27:VAL:O     | 15:AO:31:LEU:HD23   | 2.20                     | 0.41              |
| 15:AO:29:VAL:HG11  | 15:AO:67:LEU:HD21   | 2.02                     | 0.41              |
| 15:AO:82:ILE:O     | 15:AO:82:ILE:HD13   | 2.20                     | 0.41              |
| 16:AP:75:ARG:C     | 16:AP:77:ALA:N      | 2.74                     | 0.41              |
| 22:AV:69:C:O2'     | 22:AV:70:G:H5'      | 2.21                     | 0.41              |
| 22:AW:50:G:H8      | 22:AW:50:G:O5'      | 2.03                     | 0.41              |
| 24:AY:209:ALA:O    | 24:AY:211:GLU:N     | 2.54                     | 0.41              |
| 24:AY:17:ILE:HG21  | 24:AY:25:LYS:HA     | 2.01                     | 0.41              |
| 24:AY:273:LEU:HA   | 24:AY:276:VAL:CG2   | 2.50                     | 0.41              |
| 24:AY:10:LYS:HE2   | 24:AY:284:LEU:HD23  | 2.02                     | 0.41              |
| 24:AY:420:ASP:C    | 24:AY:422:GLU:N     | 2.72                     | 0.41              |
| 24:AY:434:GLU:O    | 24:AY:435:ASP:HB2   | 2.20                     | 0.41              |
| 24:AY:491:VAL:CG1  | 24:AY:492:ASP:N     | 2.83                     | 0.41              |
| 24:AY:75:LYS:O     | 24:AY:77:HIS:CD2    | 2.72                     | 0.41              |
| 25:B0:73:GLY:C     | 25:B0:75:LEU:N      | 2.71                     | 0.41              |
| 26:B1:4:VAL:HG22   | 26:B1:5:CYS:N       | 2.35                     | 0.41              |
| 27:B2:22:GLU:C     | 27:B2:24:LEU:N      | 2.74                     | 0.41              |
| 27:B2:48:HIS:CG    | 27:B2:49:LYS:N      | 2.89                     | 0.41              |
| 33:B8:49:VAL:O     | 33:B8:53:PRO:HD3    | 2.20                     | 0.41              |
| 35:BA:1314:C:OP1   | 35:BA:1315:C:OP2    | 2.38                     | 0.41              |
| 35:BA:1396:U:O2    | 35:BA:1396:U:C2'    | 2.67                     | 0.41              |
| 35:BA:1819:A:O2'   | 35:BA:1820:U:P      | 2.78                     | 0.41              |
| 35:BA:1945:G:N3    | 35:BA:1945:G:H2'    | 2.33                     | 0.41              |
| 35:BA:2072:G:C2    | 35:BA:2073:C:C2     | 3.08                     | 0.41              |
| 35:BA:2202:C:H2'   | 38:BD:151:LYS:HZ1   | 1.83                     | 0.41              |
| 35:BA:2248:C:H2'   | 35:BA:2249:U:C5'    | 2.50                     | 0.41              |
| 35:BA:2309:A:H2'   | 35:BA:2310:A:C5'    | 2.50                     | 0.41              |
| 35:BA:2317:C:O2'   | 35:BA:2318:G:H5'    | 2.20                     | 0.41              |
| 35:BA:2321:G:H2'   | 35:BA:2321:G:N3     | 2.36                     | 0.41              |
| 35:BA:2349:G:H5'   | 35:BA:2349:G:H8     | 1.85                     | 0.41              |
| 35:BA:2376:A:H2'   | 35:BA:2377:A:O4'    | 2.20                     | 0.41              |
| 35:BA:2460:U:H2'   | 35:BA:2460:U:O2     | 2.20                     | 0.41              |
| 35:BA:2513:G:C5    | 35:BA:2514:U:C4     | 3.08                     | 0.41              |
| 35:BA:2688:U:H5    | 35:BA:2720:U:OP2    | 2.03                     | 0.41              |
| 35:BA:271(M):G:C2' | 35:BA:271(N):U:H5'' | 2.50                     | 0.41              |
| 35:BA:2762:G:C5'   | 35:BA:2762:G:C8     | 3.01                     | 0.41              |
| 35:BA:2777:G:C5'   | 35:BA:2778:A:H5''   | 2.50                     | 0.41              |
| 35:BA:481:G:HO2'   | 35:BA:482:A:H8      | 1.68                     | 0.41              |
| 35:BA:654(S):G:H3' | 35:BA:654(T):C:C4'  | 2.50                     | 0.41              |
| 35:BA:775:G:C4     | 35:BA:794:G:C8      | 3.08                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:BA:856:C:H2'   | 35:BA:857:C:C6     | 2.55                     | 0.41              |
| 35:BA:877:U:C2'   | 35:BA:878:A:H5''   | 2.50                     | 0.41              |
| 37:BC:10:ALA:O    | 37:BC:13:GLU:HG2   | 2.21                     | 0.41              |
| 37:BC:226:ASN:HA  | 37:BC:227:PRO:HD2  | 1.84                     | 0.41              |
| 39:BE:31:CYS:O    | 39:BE:91:VAL:N     | 2.50                     | 0.41              |
| 40:BF:179:GLU:O   | 40:BF:181:LEU:N    | 2.53                     | 0.41              |
| 40:BF:29:ASN:HB3  | 40:BF:32:LEU:HB3   | 2.03                     | 0.41              |
| 42:BH:120:GLY:C   | 42:BH:121:ILE:HG13 | 2.40                     | 0.41              |
| 42:BH:50:VAL:CG1  | 42:BH:51:ARG:N     | 2.83                     | 0.41              |
| 43:BJ:48:UNK:O    | 43:BJ:90:UNK:CB    | 2.67                     | 0.41              |
| 44:BK:10:LEU:HD11 | 44:BK:27:LEU:HD11  | 2.02                     | 0.41              |
| 44:BK:99:ILE:HD12 | 44:BK:103:GLN:CB   | 2.47                     | 0.41              |
| 48:BP:83:VAL:H    | 48:BP:115:LEU:HD23 | 1.83                     | 0.41              |
| 50:BR:38:VAL:HB   | 50:BR:39:PRO:CD    | 2.36                     | 0.41              |
| 50:BR:78:LYS:HG2  | 50:BR:78:LYS:O     | 2.20                     | 0.41              |
| 51:BS:22:GLY:O    | 51:BS:23:ARG:O     | 2.39                     | 0.41              |
| 56:BX:53:LYS:HB3  | 56:BX:82:GLN:HB3   | 2.02                     | 0.41              |
| 58:BZ:166:SER:HB2 | 58:BZ:168:GLU:N    | 2.33                     | 0.41              |
| 1:CA:1104:G:O2'   | 1:CA:1105:A:H5'    | 2.20                     | 0.41              |
| 1:CA:1245:A:C2    | 1:CA:1293:G:C2     | 3.08                     | 0.41              |
| 1:CA:1250:A:C2    | 1:CA:1251:A:C4     | 3.08                     | 0.41              |
| 1:CA:1298:C:C2'   | 1:CA:1298:C:O2     | 2.61                     | 0.41              |
| 1:CA:1402:C:H2'   | 1:CA:1403:C:O4'    | 2.21                     | 0.41              |
| 1:CA:318:G:O2'    | 1:CA:319:G:H5'     | 2.20                     | 0.41              |
| 1:CA:913:A:H4'    | 1:CA:914:A:OP1     | 2.21                     | 0.41              |
| 1:CA:948:C:H2'    | 1:CA:949:A:C8      | 2.56                     | 0.41              |
| 2:CB:117:GLU:O    | 2:CB:120:ALA:HB3   | 2.20                     | 0.41              |
| 2:CB:23:ARG:HA    | 2:CB:23:ARG:HD2    | 1.85                     | 0.41              |
| 2:CB:44:LEU:H     | 2:CB:44:LEU:CD1    | 2.08                     | 0.41              |
| 4:CD:179:GLU:C    | 4:CD:181:MET:H     | 2.24                     | 0.41              |
| 6:CF:95:GLU:HA    | 6:CF:96:PRO:HD3    | 1.89                     | 0.41              |
| 7:CG:21:VAL:HG23  | 7:CG:22:LEU:N      | 2.36                     | 0.41              |
| 9:CI:99:LEU:HD22  | 9:CI:99:LEU:N      | 2.36                     | 0.41              |
| 12:CL:7:ILE:CG2   | 12:CL:8:ASN:N      | 2.82                     | 0.41              |
| 13:CM:16:ASP:OD2  | 13:CM:16:ASP:N     | 2.52                     | 0.41              |
| 13:CM:81:LEU:HD22 | 13:CM:81:LEU:H     | 1.82                     | 0.41              |
| 15:CO:70:LEU:HD12 | 15:CO:70:LEU:HA    | 1.90                     | 0.41              |
| 17:CQ:63:ARG:HG2  | 17:CQ:64:PRO:HD2   | 2.02                     | 0.41              |
| 18:CR:36:ASN:OD1  | 18:CR:39:VAL:HB    | 2.20                     | 0.41              |
| 22:CW:70:C:H2'    | 22:CW:71:G:O4'     | 2.20                     | 0.41              |
| 28:D3:40:THR:O    | 28:D3:44:ARG:HG3   | 2.19                     | 0.41              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:D4:28:LYS:HA   | 29:D4:28:LYS:HE3   | 2.01                     | 0.41              |
| 29:D4:30:GLU:C    | 29:D4:31:ILE:HD12  | 2.39                     | 0.41              |
| 30:D5:26:THR:HA   | 30:D5:27:PRO:HD3   | 1.96                     | 0.41              |
| 31:D6:17:LYS:CB   | 31:D6:44:ARG:NH1   | 2.83                     | 0.41              |
| 35:DA:1128:A:C8   | 35:DA:2518:A:N6    | 2.88                     | 0.41              |
| 35:DA:1156:A:O2'  | 35:DA:1157:G:OP1   | 2.34                     | 0.41              |
| 35:DA:1251:C:OP2  | 53:DU:10:ARG:NE    | 2.52                     | 0.41              |
| 35:DA:1495:A:H2'  | 35:DA:1496:A:C2    | 2.55                     | 0.41              |
| 35:DA:1499:C:C2'  | 35:DA:1500:G:H5'   | 2.50                     | 0.41              |
| 35:DA:1877:A:H5'  | 35:DA:1878:G:OP2   | 2.21                     | 0.41              |
| 35:DA:1888:G:N3   | 35:DA:1888:G:H5'   | 2.35                     | 0.41              |
| 35:DA:1902:C:H1'  | 38:DD:244:ARG:HG3  | 2.02                     | 0.41              |
| 24:CY:580:MET:SD  | 35:DA:1913:A:N6    | 2.94                     | 0.41              |
| 35:DA:1930:G:O2'  | 35:DA:1931:U:OP2   | 2.38                     | 0.41              |
| 35:DA:2078:C:C1'  | 35:DA:2434:A:H1'   | 2.51                     | 0.41              |
| 35:DA:2051:A:N6   | 35:DA:2614:A:C8    | 2.88                     | 0.41              |
| 35:DA:2624:G:O2'  | 35:DA:2625:G:H5'   | 2.20                     | 0.41              |
| 35:DA:270:A:O2'   | 35:DA:271:A:H5'    | 2.19                     | 0.41              |
| 35:DA:436:C:H2'   | 35:DA:437:G:C8     | 2.56                     | 0.41              |
| 35:DA:444:C:H2'   | 35:DA:445:C:H6     | 1.85                     | 0.41              |
| 35:DA:881:G:H2'   | 35:DA:882:G:C5'    | 2.50                     | 0.41              |
| 35:DA:8:A:H2'     | 35:DA:9:U:C6       | 2.55                     | 0.41              |
| 37:DC:119:ASP:OD1 | 37:DC:120:VAL:HG13 | 2.21                     | 0.41              |
| 37:DC:178:LYS:HG2 | 37:DC:181:PHE:CE1  | 2.55                     | 0.41              |
| 38:DD:34:VAL:O    | 38:DD:36:PRO:CD    | 2.68                     | 0.41              |
| 40:DF:10:PRO:CG   | 40:DF:13:SER:OG    | 2.69                     | 0.41              |
| 40:DF:7:TYR:CD2   | 40:DF:16:GLY:HA3   | 2.35                     | 0.41              |
| 41:DG:136:ARG:O   | 41:DG:153:ARG:O    | 2.38                     | 0.41              |
| 42:DH:124:GLU:HB2 | 42:DH:132:ARG:CG   | 2.49                     | 0.41              |
| 47:DO:31:LYS:HB3  | 47:DO:32:TYR:CE1   | 2.54                     | 0.41              |
| 50:DR:18:LEU:C    | 50:DR:20:LEU:N     | 2.74                     | 0.41              |
| 50:DR:78:LYS:O    | 50:DR:78:LYS:HG2   | 2.20                     | 0.41              |
| 50:DR:83:ILE:HG22 | 50:DR:83:ILE:O     | 2.20                     | 0.41              |
| 52:DT:120:ARG:O   | 52:DT:124:ASP:OD1  | 2.38                     | 0.41              |
| 53:DU:50:ARG:HH11 | 54:DV:70:ILE:CG2   | 2.33                     | 0.41              |
| 53:DU:76:TYR:O    | 53:DU:79:PHE:HB3   | 2.20                     | 0.41              |
| 55:DW:29:LEU:HD11 | 55:DW:51:LEU:CD1   | 2.41                     | 0.41              |
| 57:DY:99:CYS:SG   | 57:DY:99:CYS:O     | 2.79                     | 0.41              |
| 58:DZ:129:SER:CB  | 58:DZ:131:ARG:HD2  | 2.50                     | 0.41              |
| 58:DZ:4:ARG:HH12  | 58:DZ:66:SER:HB2   | 1.85                     | 0.41              |
| 58:DZ:9:TYR:CD1   | 58:DZ:35:ARG:NH1   | 2.86                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:1298:C:O2'    | 1:AA:1299:A:C2    | 2.74                     | 0.41              |
| 1:AA:1502:A:C2     | 1:AA:1505:G:N1    | 2.60                     | 0.41              |
| 1:AA:176:C:C2      | 1:AA:177:C:C5     | 3.08                     | 0.41              |
| 1:AA:238:G:O2'     | 1:AA:239:U:H5'    | 2.21                     | 0.41              |
| 1:AA:981:U:H2'     | 1:AA:982:U:C5     | 2.56                     | 0.41              |
| 2:AB:114:ARG:O     | 2:AB:117:GLU:HB2  | 2.21                     | 0.41              |
| 2:AB:17:PHE:HB3    | 2:AB:44:LEU:CD2   | 2.45                     | 0.41              |
| 2:AB:211:ILE:HG13  | 2:AB:211:ILE:H    | 1.70                     | 0.41              |
| 3:AC:90:GLU:C      | 3:AC:93:LYS:HB3   | 2.35                     | 0.41              |
| 7:AG:50:ILE:HG21   | 7:AG:58:PRO:HA    | 2.03                     | 0.41              |
| 8:AH:32:LYS:O      | 8:AH:33:GLU:C     | 2.58                     | 0.41              |
| 9:AI:51:ARG:HG3    | 9:AI:56:LEU:HD12  | 2.03                     | 0.41              |
| 10:AJ:61:GLU:OE2   | 14:AN:45:ARG:NH1  | 2.51                     | 0.41              |
| 11:AK:30:VAL:O     | 11:AK:30:VAL:HG23 | 2.21                     | 0.41              |
| 12:AL:33:ARG:CG    | 12:AL:60:LEU:HD12 | 2.50                     | 0.41              |
| 1:AA:1226:C:C4     | 13:AM:104:ARG:HB2 | 2.55                     | 0.41              |
| 16:AP:53:VAL:CG2   | 16:AP:54:GLU:H    | 2.29                     | 0.41              |
| 17:AQ:52:LYS:HD2   | 17:AQ:52:LYS:N    | 2.20                     | 0.41              |
| 17:AQ:52:LYS:CD    | 17:AQ:55:ASP:OD2  | 2.68                     | 0.41              |
| 19:AS:61:TYR:CG    | 19:AS:62:ILE:N    | 2.88                     | 0.41              |
| 20:AT:49:ALA:HB3   | 20:AT:99:LEU:CD1  | 2.50                     | 0.41              |
| 23:AX:13:A:H2'     | 23:AX:14:A:H5''   | 2.02                     | 0.41              |
| 24:AY:232:LEU:HD22 | 24:AY:232:LEU:H   | 1.84                     | 0.41              |
| 24:AY:238:THR:C    | 24:AY:240:GLU:N   | 2.74                     | 0.41              |
| 24:AY:617:MET:O    | 24:AY:618:GLY:C   | 2.57                     | 0.41              |
| 25:B0:23:VAL:HA    | 25:B0:38:VAL:HG13 | 2.03                     | 0.41              |
| 26:B1:71:TYR:HA    | 26:B1:74:VAL:HG23 | 2.03                     | 0.41              |
| 27:B2:38:GLN:CA    | 27:B2:41:ILE:HG12 | 2.50                     | 0.41              |
| 30:B5:16:ARG:HG2   | 30:B5:16:ARG:HH11 | 1.84                     | 0.41              |
| 34:B9:29:ASN:C     | 34:B9:31:LYS:H    | 2.24                     | 0.41              |
| 35:BA:1118:C:H2'   | 35:BA:1119:C:C6   | 2.56                     | 0.41              |
| 35:BA:1204:A:H1'   | 35:BA:1206:G:N7   | 2.35                     | 0.41              |
| 35:BA:1645:G:OP1   | 35:BA:1646:C:H5'  | 2.20                     | 0.41              |
| 35:BA:1676:A:H2'   | 35:BA:1677:A:O4'  | 2.20                     | 0.41              |
| 35:BA:2128:C:OP1   | 37:BC:37:LYS:N    | 2.52                     | 0.41              |
| 35:BA:2397:G:H2'   | 35:BA:2398:U:C6   | 2.56                     | 0.41              |
| 35:BA:2664:G:C2'   | 35:BA:2665:A:O5'  | 2.68                     | 0.41              |
| 35:BA:26:G:H1'     | 35:BA:515:A:N6    | 2.31                     | 0.41              |
| 35:BA:436:C:H2'    | 35:BA:437:G:C8    | 2.56                     | 0.41              |
| 35:BA:463:G:C2     | 35:BA:467:G:C6    | 3.08                     | 0.41              |
| 35:BA:760:G:H2'    | 35:BA:761:A:H5'   | 2.02                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:836:G:C5     | 35:BA:837:C:C4     | 3.08                     | 0.41              |
| 35:BA:88:G:N3      | 35:BA:88:G:H2'     | 2.36                     | 0.41              |
| 29:B4:3:GLU:CG     | 36:BB:43:C:OP1     | 2.67                     | 0.41              |
| 36:BB:4:C:H2'      | 36:BB:5:C:C6       | 2.54                     | 0.41              |
| 38:BD:21:PHE:O     | 38:BD:24:ILE:HG23  | 2.20                     | 0.41              |
| 39:BE:51:PHE:HD1   | 39:BE:52:LEU:N     | 2.16                     | 0.41              |
| 40:BF:177:ALA:HB1  | 40:BF:178:PRO:CD   | 2.50                     | 0.41              |
| 41:BG:181:ARG:HH11 | 41:BG:181:ARG:HG3  | 1.84                     | 0.41              |
| 41:BG:55:LYS:HD3   | 41:BG:55:LYS:C     | 2.41                     | 0.41              |
| 41:BG:98:ARG:N     | 41:BG:98:ARG:NH1   | 2.65                     | 0.41              |
| 42:BH:128:PRO:HG2  | 42:BH:129:THR:HG23 | 2.02                     | 0.41              |
| 42:BH:41:MET:HG3   | 42:BH:42:ARG:N     | 2.36                     | 0.41              |
| 44:BK:33:ASN:C     | 44:BK:35:MET:H     | 2.24                     | 0.41              |
| 46:BN:45:ASN:N     | 46:BN:45:ASN:ND2   | 2.54                     | 0.41              |
| 47:BO:22:ILE:O     | 47:BO:23:ARG:HB3   | 2.19                     | 0.41              |
| 49:BQ:75:THR:CG2   | 49:BQ:76:LYS:H     | 2.34                     | 0.41              |
| 35:BA:1276:A:C1'   | 50:BR:16:HIS:HE1   | 2.33                     | 0.41              |
| 51:BS:74:ALA:CB    | 51:BS:103:GLU:HB2  | 2.46                     | 0.41              |
| 51:BS:47:THR:HG22  | 51:BS:49:VAL:O     | 2.19                     | 0.41              |
| 52:BT:29:ARG:CD    | 52:BT:86:ILE:HG22  | 2.48                     | 0.41              |
| 52:BT:92:GLY:C     | 52:BT:94:ALA:H     | 2.24                     | 0.41              |
| 56:BX:63:LYS:HB3   | 56:BX:72:LYS:HG2   | 2.03                     | 0.41              |
| 57:BY:62:GLU:HG2   | 57:BY:63:LYS:N     | 2.28                     | 0.41              |
| 57:BY:96:ILE:CD1   | 57:BY:99:CYS:SG    | 3.06                     | 0.41              |
| 58:BZ:128:VAL:CG2  | 58:BZ:132:ASN:HB2  | 2.49                     | 0.41              |
| 58:BZ:24:LEU:C     | 58:BZ:24:LEU:HD23  | 2.41                     | 0.41              |
| 58:BZ:54:HIS:HA    | 58:BZ:98:MET:CE    | 2.50                     | 0.41              |
| 1:CA:1100:C:C2'    | 1:CA:1101:A:H5''   | 2.48                     | 0.41              |
| 1:CA:1103:C:C5'    | 2:CB:98:LEU:HD13   | 2.49                     | 0.41              |
| 1:CA:110:C:H2'     | 1:CA:111:G:O4'     | 2.21                     | 0.41              |
| 1:CA:1122:U:H2'    | 1:CA:1123:A:H5'    | 2.02                     | 0.41              |
| 1:CA:1347:G:H2'    | 1:CA:1373:G:H1     | 1.85                     | 0.41              |
| 1:CA:398:C:H2'     | 1:CA:399:G:C8      | 2.54                     | 0.41              |
| 2:CB:149:LEU:HD23  | 2:CB:149:LEU:HA    | 1.85                     | 0.41              |
| 3:CC:141:VAL:O     | 3:CC:144:SER:N     | 2.53                     | 0.41              |
| 3:CC:141:VAL:CG1   | 3:CC:146:ALA:HB3   | 2.51                     | 0.41              |
| 3:CC:60:ALA:N      | 3:CC:63:ASN:OD1    | 2.51                     | 0.41              |
| 3:CC:47:LEU:HD21   | 3:CC:68:VAL:HG11   | 2.02                     | 0.41              |
| 4:CD:73:ARG:HD3    | 4:CD:73:ARG:HA     | 1.76                     | 0.41              |
| 5:CE:100:VAL:O     | 5:CE:100:VAL:CG2   | 2.68                     | 0.41              |
| 7:CG:104:LEU:HA    | 7:CG:104:LEU:HD13  | 1.91                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:CG:31:MET:SD     | 7:CG:36:LYS:HB2    | 2.60                     | 0.41              |
| 7:CG:52:GLU:O      | 7:CG:53:LYS:C      | 2.58                     | 0.41              |
| 7:CG:57:GLU:O      | 7:CG:58:PRO:C      | 2.58                     | 0.41              |
| 9:CI:77:ILE:O      | 9:CI:78:LYS:C      | 2.58                     | 0.41              |
| 9:CI:90:PRO:HG2    | 9:CI:91:ASP:H      | 1.85                     | 0.41              |
| 11:CK:121:PRO:HB2  | 11:CK:126:ARG:HB2  | 2.02                     | 0.41              |
| 12:CL:20:LYS:CD    | 12:CL:20:LYS:N     | 2.83                     | 0.41              |
| 12:CL:27:LEU:C     | 12:CL:29:GLY:H     | 2.24                     | 0.41              |
| 13:CM:23:TYR:O     | 13:CM:66:LEU:HB3   | 2.20                     | 0.41              |
| 1:CA:1014:A:C2     | 19:CS:34:TRP:CE2   | 3.08                     | 0.41              |
| 20:CT:43:LEU:O     | 20:CT:44:ALA:C     | 2.58                     | 0.41              |
| 22:CV:72:A:H2'     | 22:CV:73:A:C8      | 2.56                     | 0.41              |
| 24:CY:197:ARG:O    | 24:CY:199:ILE:HG23 | 2.20                     | 0.41              |
| 24:CY:264:LEU:HD23 | 24:CY:265:LYS:HD3  | 2.02                     | 0.41              |
| 24:CY:334:THR:HG21 | 24:CY:368:GLU:HB2  | 2.02                     | 0.41              |
| 24:CY:500:GLN:HB2  | 24:CY:500:GLN:HE21 | 1.66                     | 0.41              |
| 24:CY:543:GLN:O    | 24:CY:547:GLU:HB2  | 2.20                     | 0.41              |
| 26:D1:86:SER:HB2   | 26:D1:90:ILE:CG1   | 2.47                     | 0.41              |
| 27:D2:59:ARG:HB3   | 35:DA:77:C:H5'     | 2.01                     | 0.41              |
| 28:D3:1:MET:HB3    | 28:D3:2:PRO:HD2    | 2.02                     | 0.41              |
| 28:D3:35:ARG:CD    | 28:D3:37:LEU:HD21  | 2.50                     | 0.41              |
| 31:D6:10:LEU:N     | 31:D6:10:LEU:HD23  | 2.31                     | 0.41              |
| 31:D6:27:LYS:HB3   | 31:D6:30:THR:CG2   | 2.51                     | 0.41              |
| 33:D8:19:SER:HB2   | 33:D8:21:LYS:HG3   | 2.01                     | 0.41              |
| 35:DA:1073:A:H2'   | 35:DA:1074:G:H5'   | 2.01                     | 0.41              |
| 35:DA:1131:G:N3    | 35:DA:1132:A:C8    | 2.87                     | 0.41              |
| 35:DA:1142:U:O5'   | 35:DA:1142:U:H6    | 2.04                     | 0.41              |
| 35:DA:1175:U:P     | 35:DA:1176:G:H5''  | 2.61                     | 0.41              |
| 35:DA:1203:G:OP2   | 35:DA:1204:A:H2'   | 2.21                     | 0.41              |
| 35:DA:1348:G:C3'   | 35:DA:1349:A:H5''  | 2.48                     | 0.41              |
| 35:DA:1654:A:C2    | 39:DE:113:PHE:HD1  | 2.37                     | 0.41              |
| 35:DA:1834:U:O3'   | 35:DA:1835:G:H8    | 2.04                     | 0.41              |
| 35:DA:2154:G:H21   | 35:DA:2155:G:H1'   | 1.86                     | 0.41              |
| 35:DA:2103:C:N4    | 35:DA:2186:G:H1    | 2.19                     | 0.41              |
| 35:DA:2543:G:O2'   | 35:DA:2544:G:H5'   | 2.21                     | 0.41              |
| 35:DA:272(J):C:N4  | 35:DA:363:G:H22    | 2.19                     | 0.41              |
| 32:D7:39:ARG:NH2   | 35:DA:468:G:N7     | 2.63                     | 0.41              |
| 35:DA:603:A:O2'    | 35:DA:604:G:OP2    | 2.35                     | 0.41              |
| 35:DA:669:G:C2'    | 35:DA:669:G:N3     | 2.84                     | 0.41              |
| 35:DA:88:G:OP1     | 35:DA:90:U:C5      | 2.63                     | 0.41              |
| 35:DA:948:G:OP1    | 35:DA:962:G:OP1    | 2.39                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:DA:968:G:C6    | 35:DA:969:U:C4     | 3.08                     | 0.41              |
| 36:DB:18:G:H2'    | 36:DB:19:G:C8      | 2.50                     | 0.41              |
| 22:CW:19:G:OP1    | 37:DC:168:LYS:NZ   | 2.54                     | 0.41              |
| 38:DD:34:VAL:O    | 38:DD:36:PRO:HD2   | 2.21                     | 0.41              |
| 39:DE:131:ALA:HB3 | 39:DE:134:ILE:CD1  | 2.17                     | 0.41              |
| 40:DF:102:PRO:HB2 | 40:DF:105:VAL:HG23 | 2.01                     | 0.41              |
| 40:DF:117:ARG:NH1 | 40:DF:120:GLU:OE1  | 2.53                     | 0.41              |
| 41:DG:11:TYR:OH   | 41:DG:33:ARG:HB3   | 2.20                     | 0.41              |
| 42:DH:130:ARG:HB3 | 42:DH:130:ARG:NH1  | 2.35                     | 0.41              |
| 43:DJ:50:UNK:O    | 43:DJ:51:UNK:CB    | 2.68                     | 0.41              |
| 48:DP:47:ASP:CB   | 48:DP:48:PRO:CA    | 2.93                     | 0.41              |
| 50:DR:52:ILE:HG21 | 50:DR:94:TYR:CG    | 2.55                     | 0.41              |
| 51:DS:63:THR:O    | 51:DS:66:ALA:N     | 2.53                     | 0.41              |
| 52:DT:2:ASN:O     | 52:DT:4:GLY:N      | 2.53                     | 0.41              |
| 52:DT:78:LEU:HB3  | 52:DT:79:HIS:ND1   | 2.35                     | 0.41              |
| 57:DY:90:LEU:HB2  | 57:DY:91:GLU:OE2   | 2.20                     | 0.41              |
| 58:DZ:120:ILE:CG2 | 58:DZ:120:ILE:O    | 2.67                     | 0.41              |
| 1:AA:1202:G:H2'   | 1:AA:1203:C:C5'    | 2.51                     | 0.41              |
| 1:AA:1511:G:C6    | 1:AA:1512:U:C4     | 3.08                     | 0.41              |
| 1:AA:318:G:C2     | 1:AA:336:C:N3      | 2.88                     | 0.41              |
| 1:AA:51:A:H4'     | 1:AA:52:G:C5'      | 2.51                     | 0.41              |
| 2:AB:17:PHE:HD2   | 2:AB:17:PHE:H      | 1.69                     | 0.41              |
| 2:AB:229:VAL:CG1  | 2:AB:230:VAL:N     | 2.83                     | 0.41              |
| 3:AC:206:GLU:O    | 3:AC:208:ILE:N     | 2.53                     | 0.41              |
| 4:AD:68:TYR:O     | 4:AD:69:GLY:C      | 2.59                     | 0.41              |
| 4:AD:205:GLU:OE1  | 5:AE:100:VAL:HG22  | 2.20                     | 0.41              |
| 7:AG:146:GLU:OE2  | 7:AG:149:ARG:HD2   | 2.20                     | 0.41              |
| 7:AG:21:VAL:HG23  | 7:AG:22:LEU:H      | 1.85                     | 0.41              |
| 7:AG:61:VAL:O     | 7:AG:64:GLN:HB3    | 2.20                     | 0.41              |
| 5:AE:143:ARG:NH1  | 8:AH:77:GLU:CD     | 2.74                     | 0.41              |
| 9:AI:35:GLU:HA    | 9:AI:38:GLN:HB2    | 2.01                     | 0.41              |
| 13:AM:23:TYR:O    | 13:AM:66:LEU:HB3   | 2.20                     | 0.41              |
| 13:AM:89:GLY:O    | 13:AM:90:LEU:O     | 2.39                     | 0.41              |
| 16:AP:75:ARG:O    | 16:AP:77:ALA:N     | 2.52                     | 0.41              |
| 20:AT:44:ALA:O    | 20:AT:92:LEU:HD23  | 2.20                     | 0.41              |
| 22:AW:55:5MU:H2'  | 22:AW:56:U:C6      | 2.55                     | 0.41              |
| 24:AY:111:SER:OG  | 24:AY:141:LYS:HB3  | 2.20                     | 0.41              |
| 24:AY:20:HIS:CG   | 24:AY:117:GLN:HB3  | 2.55                     | 0.41              |
| 24:AY:117:GLN:O   | 24:AY:117:GLN:OE1  | 2.38                     | 0.41              |
| 24:AY:124:GLN:HA  | 24:AY:127:LYS:HD2  | 2.03                     | 0.41              |
| 24:AY:16:GLY:N    | 24:AY:101:LEU:CD1  | 2.83                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:AY:289:ILE:HD11 | 24:AY:331:TYR:CZ   | 2.55                     | 0.41              |
| 24:AY:590:ILE:C    | 24:AY:592:GLU:N    | 2.73                     | 0.41              |
| 24:AY:622:GLY:O    | 24:AY:623:ASP:C    | 2.58                     | 0.41              |
| 26:B1:4:VAL:CG2    | 26:B1:10:LYS:O     | 2.66                     | 0.41              |
| 26:B1:90:ILE:HG22  | 26:B1:94:LEU:HD11  | 2.02                     | 0.41              |
| 27:B2:58:ALA:O     | 27:B2:62:THR:N     | 2.48                     | 0.41              |
| 35:BA:118:A:H5'    | 35:BA:119:A:H8     | 1.86                     | 0.41              |
| 35:BA:1741:A:H2'   | 35:BA:1742:G:O4'   | 2.20                     | 0.41              |
| 35:BA:1956:U:C2'   | 35:BA:1957:C:H5'   | 2.50                     | 0.41              |
| 35:BA:2288:A:C2    | 35:BA:2325:G:N7    | 2.88                     | 0.41              |
| 35:BA:2455:G:H2'   | 35:BA:2456:C:H6    | 1.79                     | 0.41              |
| 35:BA:2557:G:H2'   | 35:BA:2558:C:C6    | 2.55                     | 0.41              |
| 35:BA:2786:U:O2'   | 39:BE:62:PRO:HA    | 2.21                     | 0.41              |
| 35:BA:301:G:C4     | 35:BA:302:C:C5     | 3.09                     | 0.41              |
| 35:BA:664:C:H4'    | 35:BA:941:A:OP1    | 2.19                     | 0.41              |
| 37:BC:139:PRO:HA   | 37:BC:145:THR:HG21 | 2.03                     | 0.41              |
| 37:BC:48:LEU:N     | 37:BC:48:LEU:CD1   | 2.82                     | 0.41              |
| 38:BD:245:PRO:O    | 38:BD:245:PRO:HG2  | 2.20                     | 0.41              |
| 39:BE:25:VAL:HG22  | 39:BE:183:LEU:HG   | 2.02                     | 0.41              |
| 40:BF:132:VAL:CG2  | 40:BF:133:ASN:H    | 2.29                     | 0.41              |
| 41:BG:15:VAL:HG22  | 41:BG:175:LEU:O    | 2.20                     | 0.41              |
| 42:BH:35:VAL:HG21  | 42:BH:75:ALA:CB    | 2.51                     | 0.41              |
| 44:BK:30:HIS:CA    | 44:BK:59:ILE:HD12  | 2.39                     | 0.41              |
| 48:BP:98:GLU:H     | 48:BP:101:VAL:HG13 | 1.86                     | 0.41              |
| 35:BA:2000:G:OP2   | 50:BR:3:HIS:HE1    | 2.03                     | 0.41              |
| 50:BR:41:ALA:C     | 50:BR:43:GLU:H     | 2.22                     | 0.41              |
| 50:BR:55:ALA:HB2   | 50:BR:79:LEU:CD1   | 2.49                     | 0.41              |
| 51:BS:63:THR:O     | 51:BS:64:GLU:C     | 2.59                     | 0.41              |
| 52:BT:100:TYR:CD1  | 52:BT:100:TYR:N    | 2.89                     | 0.41              |
| 53:BU:92:ARG:NH1   | 54:BV:11:GLN:CG    | 2.82                     | 0.41              |
| 58:BZ:81:ARG:CZ    | 58:BZ:81:ARG:HB3   | 2.50                     | 0.41              |
| 1:CA:1061:G:H1'    | 10:CJ:56:HIS:CE1   | 2.56                     | 0.41              |
| 1:CA:1347:G:H1'    | 1:CA:1348:U:H5     | 1.86                     | 0.41              |
| 1:CA:1505:G:H5'    | 1:CA:1506:U:OP1    | 2.20                     | 0.41              |
| 1:CA:151:A:H2'     | 1:CA:152:A:H5'     | 2.02                     | 0.41              |
| 1:CA:253:U:H2'     | 1:CA:254:G:C8      | 2.55                     | 0.41              |
| 1:CA:44:G:C2       | 1:CA:45:U:H1'      | 2.55                     | 0.41              |
| 1:CA:955:U:H2'     | 1:CA:956:U:C6      | 2.56                     | 0.41              |
| 2:CB:160:ASP:O     | 2:CB:161:ALA:HB2   | 2.20                     | 0.41              |
| 2:CB:12:GLU:CA     | 2:CB:16:HIS:ND1    | 2.83                     | 0.41              |
| 2:CB:21:ARG:O      | 2:CB:22:LYS:HB2    | 2.20                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:CD:11:LEU:C     | 4:CD:13:ARG:N      | 2.69                     | 0.41              |
| 5:CE:12:LEU:CD1   | 5:CE:31:LEU:CB     | 2.99                     | 0.41              |
| 6:CF:29:ALA:O     | 6:CF:30:LEU:C      | 2.59                     | 0.41              |
| 8:CH:38:ILE:O     | 8:CH:39:LEU:C      | 2.58                     | 0.41              |
| 9:CI:114:TYR:O    | 9:CI:114:TYR:CD2   | 2.74                     | 0.41              |
| 9:CI:97:LYS:N     | 9:CI:98:PRO:CD     | 2.83                     | 0.41              |
| 10:CJ:32:ALA:HB1  | 10:CJ:76:ASN:HB3   | 2.01                     | 0.41              |
| 14:CN:32:SER:O    | 14:CN:40:CYS:HA    | 2.20                     | 0.41              |
| 19:CS:9:VAL:C     | 19:CS:11:VAL:N     | 2.73                     | 0.41              |
| 19:CS:19:VAL:HG12 | 19:CS:20:LEU:N     | 2.34                     | 0.41              |
| 1:CA:1318:A:C1'   | 19:CS:37:ARG:NH2   | 2.74                     | 0.41              |
| 20:CT:54:LYS:HA   | 20:CT:57:ARG:NH2   | 2.35                     | 0.41              |
| 20:CT:73:HIS:O    | 20:CT:74:LYS:O     | 2.37                     | 0.41              |
| 20:CT:44:ALA:HA   | 20:CT:92:LEU:HD21  | 2.02                     | 0.41              |
| 24:CY:415:PRO:CG  | 24:CY:421:GLN:HG2  | 2.51                     | 0.41              |
| 24:CY:670:VAL:HB  | 24:CY:672:PHE:CE1  | 2.54                     | 0.41              |
| 30:D5:2:ALA:HB2   | 35:DA:2015:A:O4'   | 2.20                     | 0.41              |
| 31:D6:29:ASN:O    | 31:D6:30:THR:C     | 2.59                     | 0.41              |
| 31:D6:41:PRO:HD3  | 31:D6:47:THR:HG22  | 2.01                     | 0.41              |
| 33:D8:62:LEU:HD13 | 35:DA:242:G:C5'    | 2.43                     | 0.41              |
| 35:DA:1038:C:H3'  | 35:DA:1039:G:C5'   | 2.36                     | 0.41              |
| 35:DA:1317:A:H2'  | 35:DA:1318:C:H6    | 1.85                     | 0.41              |
| 35:DA:152:G:H1    | 35:DA:174:C:H42    | 1.68                     | 0.41              |
| 35:DA:1430:C:H42  | 35:DA:1563:G:H1    | 1.68                     | 0.41              |
| 1:CA:1495:U:O2'   | 35:DA:1919:A:N1    | 2.48                     | 0.41              |
| 35:DA:1948:G:H8   | 35:DA:1948:G:C5'   | 2.32                     | 0.41              |
| 30:D5:2:ALA:N     | 35:DA:2015:A:C1'   | 2.83                     | 0.41              |
| 35:DA:28:A:H1'    | 35:DA:513:A:C2     | 2.56                     | 0.41              |
| 35:DA:36:G:H2'    | 35:DA:37:C:H6      | 1.85                     | 0.41              |
| 35:DA:414:C:O2    | 35:DA:1864:U:O2'   | 2.26                     | 0.41              |
| 35:DA:750:A:C3'   | 35:DA:751:A:H5''   | 2.50                     | 0.41              |
| 36:DB:81:G:O6     | 36:DB:96:U:O2      | 2.38                     | 0.41              |
| 37:DC:115:VAL:CG1 | 37:DC:145:THR:HG23 | 2.47                     | 0.41              |
| 35:DA:729:G:C5    | 38:DD:208:LYS:HB2  | 2.55                     | 0.41              |
| 38:DD:28:GLU:CD   | 38:DD:28:GLU:N     | 2.73                     | 0.41              |
| 35:DA:1568:G:H4'  | 38:DD:59:LYS:HB3   | 2.02                     | 0.41              |
| 39:DE:7:VAL:HG13  | 39:DE:7:VAL:O      | 2.20                     | 0.41              |
| 40:DF:28:ILE:N    | 40:DF:28:ILE:CD1   | 2.83                     | 0.41              |
| 40:DF:31:HIS:O    | 40:DF:32:LEU:C     | 2.59                     | 0.41              |
| 41:DG:55:LYS:O    | 41:DG:57:ALA:N     | 2.53                     | 0.41              |
| 42:DH:173:PRO:HG2 | 42:DH:174:GLY:H    | 1.85                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 42:DH:92:ILE:HG22 | 42:DH:93:GLY:N    | 2.36                     | 0.41              |
| 47:DO:112:MET:O   | 47:DO:113:LYS:C   | 2.58                     | 0.41              |
| 40:DF:187:VAL:CG1 | 48:DP:7:ARG:NH2   | 2.83                     | 0.41              |
| 50:DR:28:LEU:HD23 | 50:DR:29:LEU:HD12 | 2.00                     | 0.41              |
| 53:DU:57:PHE:O    | 53:DU:59:ARG:N    | 2.54                     | 0.41              |
| 57:DY:44:ILE:O    | 57:DY:62:GLU:HB3  | 2.20                     | 0.41              |
| 58:DZ:128:VAL:CG1 | 58:DZ:132:ASN:O   | 2.69                     | 0.41              |
| 58:DZ:14:LYS:HB2  | 58:DZ:17:ALA:CB   | 2.50                     | 0.41              |
| 1:AA:1122:U:H2'   | 1:AA:1123:A:C5'   | 2.50                     | 0.41              |
| 1:AA:1248:A:C5    | 1:AA:1249:C:C5    | 3.08                     | 0.41              |
| 1:AA:791:G:N2     | 1:AA:1497:G:O3'   | 2.48                     | 0.41              |
| 2:AB:39:ILE:O     | 2:AB:41:ILE:HD13  | 2.20                     | 0.41              |
| 2:AB:7:VAL:O      | 2:AB:11:LEU:CG    | 2.69                     | 0.41              |
| 3:AC:77:ILE:O     | 3:AC:84:ILE:HG22  | 2.20                     | 0.41              |
| 1:AA:1343:G:H1'   | 9:AI:121:ARG:HH12 | 1.86                     | 0.41              |
| 9:AI:50:LEU:C     | 9:AI:52:ALA:N     | 2.74                     | 0.41              |
| 11:AK:120:ARG:HA  | 11:AK:121:PRO:HD3 | 1.82                     | 0.41              |
| 12:AL:7:ILE:HA    | 12:AL:10:LEU:HD12 | 2.03                     | 0.41              |
| 13:AM:40:ASN:HD21 | 13:AM:42:ALA:HB3  | 1.86                     | 0.41              |
| 15:AO:83:GLU:C    | 15:AO:85:LEU:N    | 2.69                     | 0.41              |
| 15:AO:83:GLU:O    | 15:AO:85:LEU:N    | 2.52                     | 0.41              |
| 17:AQ:26:GLN:HG2  | 17:AQ:37:LYS:HG3  | 2.02                     | 0.41              |
| 20:AT:38:LYS:O    | 20:AT:40:ALA:N    | 2.52                     | 0.41              |
| 21:AU:2:GLY:C     | 21:AU:4:GLY:H     | 2.24                     | 0.41              |
| 22:AV:30:G:N2     | 22:AV:31:G:H1'    | 2.36                     | 0.41              |
| 26:B1:8:SER:HB3   | 26:B1:66:HIS:CG   | 2.56                     | 0.41              |
| 27:B2:20:GLU:C    | 27:B2:20:GLU:OE1  | 2.59                     | 0.41              |
| 29:B4:27:THR:O    | 29:B4:28:LYS:CB   | 2.69                     | 0.41              |
| 35:BA:1052:C:O2'  | 35:BA:1053:C:P    | 2.78                     | 0.41              |
| 35:BA:120:U:C5'   | 35:BA:121:G:OP1   | 2.68                     | 0.41              |
| 35:BA:1235:G:C2   | 35:BA:1236:G:N2   | 2.88                     | 0.41              |
| 32:B7:48:LYS:NZ   | 35:BA:125:G:H21   | 2.18                     | 0.41              |
| 35:BA:1415:U:H3   | 35:BA:1587:A:H61  | 1.67                     | 0.41              |
| 35:BA:1495:A:H2'  | 35:BA:1496:A:C2   | 2.55                     | 0.41              |
| 35:BA:17:G:H4'    | 53:BU:25:TRP:CH2  | 2.54                     | 0.41              |
| 35:BA:1856:G:H1   | 35:BA:1886:C:N4   | 2.18                     | 0.41              |
| 35:BA:212:G:O2'   | 35:BA:213:A:H5'   | 2.21                     | 0.41              |
| 35:BA:2154:G:H21  | 35:BA:2155:G:H1'  | 1.85                     | 0.41              |
| 35:BA:2345:G:H5'  | 35:BA:2346:A:H5'  | 2.03                     | 0.41              |
| 35:BA:2380:C:C4   | 35:BA:2381:C:C5   | 3.09                     | 0.41              |
| 35:BA:2593:U:C2   | 35:BA:2594:C:C5   | 3.09                     | 0.41              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:BA:343:C:O2'   | 35:BA:344:G:H5'   | 2.20                     | 0.41              |
| 35:BA:541:C:H42   | 35:BA:552:G:H1    | 1.67                     | 0.41              |
| 35:BA:688:U:H2'   | 35:BA:689:A:C8    | 2.56                     | 0.41              |
| 35:BA:881:G:H2'   | 35:BA:882:G:C5'   | 2.51                     | 0.41              |
| 35:BA:960:A:C8    | 35:BA:962:G:C8    | 3.09                     | 0.41              |
| 37:BC:19:LYS:HG2  | 37:BC:20:VAL:N    | 2.36                     | 0.41              |
| 38:BD:166:GLN:CA  | 38:BD:166:GLN:NE2 | 2.82                     | 0.41              |
| 39:BE:132:HIS:HA  | 39:BE:135:HIS:CE1 | 2.56                     | 0.41              |
| 39:BE:152:LYS:HG3 | 39:BE:153:GLY:H   | 1.85                     | 0.41              |
| 40:BF:184:TYR:O   | 40:BF:188:ARG:HG2 | 2.21                     | 0.41              |
| 40:BF:31:HIS:O    | 40:BF:34:TRP:HB3  | 2.20                     | 0.41              |
| 40:BF:78:ILE:H    | 40:BF:78:ILE:HG12 | 1.64                     | 0.41              |
| 41:BG:27:ASN:HB3  | 41:BG:30:GLU:HB2  | 2.03                     | 0.41              |
| 42:BH:169:VAL:O   | 42:BH:170:ARG:CG  | 2.68                     | 0.41              |
| 42:BH:17:VAL:O    | 42:BH:45:VAL:CG2  | 2.62                     | 0.41              |
| 44:BK:12:LEU:HA   | 44:BK:13:PRO:HD3  | 1.85                     | 0.41              |
| 46:BN:56:ASN:HA   | 46:BN:125:GLY:N   | 2.36                     | 0.41              |
| 48:BP:88:LEU:HD11 | 48:BP:95:VAL:HG11 | 2.02                     | 0.41              |
| 49:BQ:120:ILE:O   | 49:BQ:121:ALA:C   | 2.58                     | 0.41              |
| 53:BU:13:LYS:O    | 53:BU:17:ILE:HG13 | 2.21                     | 0.41              |
| 53:BU:25:TRP:CD1  | 53:BU:26:GLY:N    | 2.89                     | 0.41              |
| 53:BU:37:GLU:O    | 53:BU:40:PHE:HB2  | 2.21                     | 0.41              |
| 35:BA:559:G:N2    | 53:BU:49:HIS:CD2  | 2.85                     | 0.41              |
| 53:BU:53:ARG:O    | 53:BU:54:LYS:C    | 2.57                     | 0.41              |
| 53:BU:55:ARG:HA   | 53:BU:58:ARG:CB   | 2.50                     | 0.41              |
| 55:BW:12:ILE:HG13 | 55:BW:42:ARG:HH11 | 1.84                     | 0.41              |
| 35:BA:748:G:C8    | 55:BW:89:ALA:HB1  | 2.56                     | 0.41              |
| 57:BY:20:TYR:CD1  | 57:BY:20:TYR:N    | 2.88                     | 0.41              |
| 1:CA:1001(A):G:H8 | 1:CA:1002:G:C8    | 2.38                     | 0.41              |
| 1:CA:1026:G:H3'   | 1:CA:1027:C:H5'   | 2.02                     | 0.41              |
| 1:CA:1145:C:H6    | 1:CA:1145:C:H5''  | 1.86                     | 0.41              |
| 1:CA:1216:G:H2'   | 1:CA:1217:C:H6    | 1.84                     | 0.41              |
| 1:CA:1305:G:H22   | 1:CA:1331:G:C2'   | 2.33                     | 0.41              |
| 1:CA:1435:G:H2'   | 1:CA:1436:U:C6    | 2.55                     | 0.41              |
| 1:CA:102:G:N3     | 1:CA:151:A:H2     | 2.19                     | 0.41              |
| 1:CA:297:G:N2     | 1:CA:299:G:H3'    | 2.36                     | 0.41              |
| 1:CA:335:C:O2'    | 1:CA:336:C:H5'    | 2.20                     | 0.41              |
| 1:CA:532:A:O2'    | 1:CA:533:A:P      | 2.79                     | 0.41              |
| 1:CA:674:G:O4'    | 18:CR:81:PHE:CE1  | 2.73                     | 0.41              |
| 1:CA:946:A:H3'    | 1:CA:947:G:C8     | 2.55                     | 0.41              |
| 1:CA:946:A:C2     | 1:CA:947:G:C5     | 3.08                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:973:G:O4'     | 10:CJ:55:LYS:CG    | 2.60                     | 0.41              |
| 3:CC:127:ARG:NH1   | 3:CC:127:ARG:HG2   | 2.36                     | 0.41              |
| 3:CC:76:VAL:HG23   | 3:CC:77:ILE:HG13   | 2.02                     | 0.41              |
| 1:CA:408:A:H4'     | 4:CD:112:VAL:HG11  | 2.01                     | 0.41              |
| 1:CA:429:U:OP1     | 4:CD:9:CYS:O       | 2.39                     | 0.41              |
| 6:CF:20:ALA:O      | 6:CF:21:LEU:C      | 2.59                     | 0.41              |
| 10:CJ:28:ARG:NH1   | 10:CJ:28:ARG:HG2   | 2.36                     | 0.41              |
| 10:CJ:4:ILE:HD13   | 10:CJ:74:ILE:CG1   | 2.43                     | 0.41              |
| 11:CK:48:ILE:N     | 11:CK:48:ILE:CD1   | 2.79                     | 0.41              |
| 11:CK:58:PRO:O     | 11:CK:59:TYR:C     | 2.58                     | 0.41              |
| 13:CM:119:GLY:C    | 13:CM:121:LYS:H    | 2.23                     | 0.41              |
| 14:CN:12:ARG:CB    | 14:CN:12:ARG:NH1   | 2.83                     | 0.41              |
| 17:CQ:8:GLY:O      | 17:CQ:56:VAL:HA    | 2.21                     | 0.41              |
| 20:CT:26:ASN:HD22  | 20:CT:27:LYS:N     | 2.18                     | 0.41              |
| 22:CW:69:C:H2'     | 22:CW:70:C:C6      | 2.55                     | 0.41              |
| 24:CY:142:THR:C    | 24:CY:144:ALA:N    | 2.74                     | 0.41              |
| 24:CY:274:ASP:O    | 24:CY:277:VAL:HG12 | 2.20                     | 0.41              |
| 24:CY:546:ILE:HG21 | 24:CY:565:VAL:HG21 | 2.02                     | 0.41              |
| 29:D4:31:ILE:O     | 29:D4:31:ILE:HG22  | 2.20                     | 0.41              |
| 31:D6:7:ILE:HG23   | 31:D6:29:ASN:HD22  | 1.85                     | 0.41              |
| 31:D6:43:CYS:O     | 31:D6:44:ARG:CB    | 2.64                     | 0.41              |
| 31:D6:53:LYS:HG3   | 31:D6:54:ILE:H     | 1.85                     | 0.41              |
| 35:DA:1034:G:C6    | 35:DA:1035:U:N3    | 2.88                     | 0.41              |
| 35:DA:1052:C:O2'   | 35:DA:1053:C:P     | 2.79                     | 0.41              |
| 35:DA:1118:C:H2'   | 35:DA:1119:C:C6    | 2.56                     | 0.41              |
| 35:DA:1314:C:C6    | 35:DA:1314:C:H5'   | 2.37                     | 0.41              |
| 35:DA:1572:A:O2'   | 35:DA:1573:G:H5'   | 2.20                     | 0.41              |
| 35:DA:688:U:H5'    | 35:DA:1780:A:H2    | 1.85                     | 0.41              |
| 35:DA:2388:A:H5'   | 35:DA:2389:G:OP2   | 2.20                     | 0.41              |
| 35:DA:2579:C:H2'   | 35:DA:2580:U:O4'   | 2.20                     | 0.41              |
| 35:DA:532:A:N1     | 35:DA:2020:A:H1'   | 2.35                     | 0.41              |
| 35:DA:603:A:O2'    | 35:DA:604:G:P      | 2.79                     | 0.41              |
| 35:DA:654(E):G:H2' | 35:DA:654(F):C:H5' | 2.03                     | 0.41              |
| 35:DA:733:G:C6     | 35:DA:761:A:C8     | 3.08                     | 0.41              |
| 35:DA:764:A:C5     | 38:DD:209:ALA:HB1  | 2.55                     | 0.41              |
| 35:DA:862:G:H2'    | 35:DA:863:A:O4'    | 2.19                     | 0.41              |
| 35:DA:94:C:O2      | 35:DA:94:C:H2'     | 2.20                     | 0.41              |
| 37:DC:114:VAL:O    | 37:DC:139:PRO:HG3  | 2.21                     | 0.41              |
| 38:DD:158:ALA:O    | 38:DD:196:VAL:CG1  | 2.67                     | 0.41              |
| 38:DD:177:LEU:O    | 38:DD:179:SER:N    | 2.54                     | 0.41              |
| 39:DE:59:VAL:HG11  | 39:DE:63:LEU:HA    | 2.02                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:DF:157:VAL:CG2 | 40:DF:194:MET:HA   | 2.50                     | 0.41              |
| 43:DJ:128:UNK:C   | 43:DJ:130:UNK:N    | 2.81                     | 0.41              |
| 44:DK:10:LEU:HD11 | 44:DK:27:LEU:HD11  | 2.01                     | 0.41              |
| 44:DK:125:ARG:HG2 | 44:DK:125:ARG:HH11 | 1.85                     | 0.41              |
| 44:DK:33:ASN:C    | 44:DK:35:MET:H     | 2.23                     | 0.41              |
| 46:DN:91:LEU:HD21 | 46:DN:98:VAL:HG11  | 2.02                     | 0.41              |
| 47:DO:53:LYS:O    | 47:DO:54:GLU:C     | 2.59                     | 0.41              |
| 47:DO:69:ILE:HB   | 47:DO:77:ILE:CG2   | 2.51                     | 0.41              |
| 48:DP:147:LEU:C   | 48:DP:148:LEU:HD12 | 2.41                     | 0.41              |
| 49:DQ:76:LYS:CB   | 49:DQ:91:GLU:HG3   | 2.49                     | 0.41              |
| 50:DR:117:VAL:CG1 | 50:DR:118:GLU:H    | 2.32                     | 0.41              |
| 50:DR:45:ARG:O    | 50:DR:46:GLY:C     | 2.59                     | 0.41              |
| 52:DT:8:LYS:C     | 52:DT:10:VAL:H     | 2.24                     | 0.41              |
| 54:DV:1:MET:HB3   | 54:DV:2:PHE:H      | 1.52                     | 0.41              |
| 57:DY:11:ASP:O    | 57:DY:27:VAL:HA    | 2.21                     | 0.41              |
| 58:DZ:44:PHE:CZ   | 58:DZ:48:PHE:HD2   | 2.39                     | 0.41              |
| 1:AA:1103:C:C5'   | 2:AB:98:LEU:HD13   | 2.51                     | 0.41              |
| 1:AA:1372:U:OP1   | 9:AI:71:SER:HB3    | 2.20                     | 0.41              |
| 1:AA:1409:C:H2'   | 1:AA:1410:G:C8     | 2.51                     | 0.41              |
| 1:AA:224:C:H2'    | 1:AA:225:C:H6      | 1.85                     | 0.41              |
| 1:AA:251:G:H4'    | 1:AA:252:U:O5'     | 2.19                     | 0.41              |
| 1:AA:425:G:O2'    | 1:AA:426:G:H5'     | 2.21                     | 0.41              |
| 1:AA:822:C:O2'    | 1:AA:823:G:H5'     | 2.20                     | 0.41              |
| 2:AB:156:LYS:O    | 2:AB:157:ARG:CB    | 2.66                     | 0.41              |
| 2:AB:220:ASP:O    | 2:AB:222:ILE:N     | 2.54                     | 0.41              |
| 3:AC:43:LEU:C     | 3:AC:45:LYS:N      | 2.73                     | 0.41              |
| 1:AA:409:G:H5'    | 4:AD:24:GLU:OE1    | 2.20                     | 0.41              |
| 5:AE:26:PHE:CD1   | 5:AE:26:PHE:N      | 2.88                     | 0.41              |
| 7:AG:134:ALA:O    | 7:AG:135:VAL:C     | 2.57                     | 0.41              |
| 9:AI:37:PHE:HB3   | 9:AI:43:ALA:HB2    | 2.02                     | 0.41              |
| 1:AA:1458:G:OP1   | 20:AT:35:THR:HG21  | 2.21                     | 0.41              |
| 22:AV:5:G:O2'     | 22:AV:6:G:H5'      | 2.20                     | 0.41              |
| 22:AV:68:C:O5'    | 22:AV:68:C:H6      | 2.02                     | 0.41              |
| 22:AW:28:U:O2'    | 22:AW:29:C:H5'     | 2.21                     | 0.41              |
| 24:AY:170:ARG:O   | 24:AY:171:GLU:CG   | 2.59                     | 0.41              |
| 24:AY:491:VAL:CG1 | 24:AY:492:ASP:H    | 2.33                     | 0.41              |
| 24:AY:519:ARG:NH2 | 24:AY:678:GLU:H    | 2.19                     | 0.41              |
| 25:B0:49:LYS:H    | 25:B0:80:HIS:HD1   | 1.68                     | 0.41              |
| 26:B1:12:PRO:HG3  | 35:BA:1365:A:H5''  | 2.02                     | 0.41              |
| 26:B1:84:GLY:O    | 26:B1:86:SER:OG    | 2.32                     | 0.41              |
| 27:B2:38:GLN:NE2  | 27:B2:44:LEU:CB    | 2.84                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:B3:15:TYR:HD1   | 28:B3:15:TYR:H     | 1.68                     | 0.41              |
| 28:B3:22:ALA:HA    | 28:B3:46:ASN:ND2   | 2.34                     | 0.41              |
| 29:B4:39:CYS:SG    | 29:B4:42:PHE:CE2   | 3.08                     | 0.41              |
| 30:B5:2:ALA:O      | 30:B5:3:LYS:CB     | 2.67                     | 0.41              |
| 32:B7:26:GLY:O     | 32:B7:30:VAL:HG23  | 2.21                     | 0.41              |
| 35:BA:1114:G:H2'   | 35:BA:1115:G:C5'   | 2.50                     | 0.41              |
| 35:BA:1142:U:H6    | 35:BA:1142:U:O5'   | 2.03                     | 0.41              |
| 35:BA:1187:G:H5''  | 54:BV:81:TYR:CE2   | 2.55                     | 0.41              |
| 35:BA:1658:C:C2    | 35:BA:1659:U:C5    | 3.08                     | 0.41              |
| 35:BA:1825:A:OP1   | 38:BD:249:PRO:HD3  | 2.20                     | 0.41              |
| 35:BA:2287:A:H2    | 35:BA:2346:A:C2    | 2.37                     | 0.41              |
| 35:BA:2393:A:O2'   | 35:BA:2394:C:H5'   | 2.20                     | 0.41              |
| 35:BA:2453:A:O2'   | 35:BA:2454:G:H5'   | 2.21                     | 0.41              |
| 35:BA:2507:C:C2    | 35:BA:2583:G:C2    | 3.09                     | 0.41              |
| 35:BA:332:A:H4'    | 35:BA:333:G:OP1    | 2.20                     | 0.41              |
| 35:BA:832:G:OP1    | 48:BP:40:SER:HB3   | 2.21                     | 0.41              |
| 35:BA:972:G:OP2    | 35:BA:974:G:H5''   | 2.20                     | 0.41              |
| 36:BB:63:G:C2      | 36:BB:64:C:C2      | 3.09                     | 0.41              |
| 37:BC:111:PHE:CE1  | 37:BC:137:LEU:HD13 | 2.39                     | 0.41              |
| 40:BF:201:VAL:HA   | 40:BF:204:ASN:HD22 | 1.86                     | 0.41              |
| 40:BF:107:LYS:HD2  | 40:BF:205:ARG:O    | 2.21                     | 0.41              |
| 40:BF:39:TRP:CH2   | 40:BF:106:ARG:NE   | 2.81                     | 0.41              |
| 41:BG:42:GLY:C     | 41:BG:43:LEU:HD22  | 2.41                     | 0.41              |
| 41:BG:55:LYS:C     | 41:BG:57:ALA:H     | 2.22                     | 0.41              |
| 41:BG:73:ALA:H     | 41:BG:87:PRO:CD    | 2.32                     | 0.41              |
| 44:BK:10:LEU:HD11  | 44:BK:27:LEU:CD1   | 2.51                     | 0.41              |
| 45:BL:67:UNK:C     | 45:BL:69:UNK:N     | 2.83                     | 0.41              |
| 46:BN:120:LEU:HD11 | 46:BN:122:VAL:CG2  | 2.50                     | 0.41              |
| 46:BN:67:LEU:HD22  | 46:BN:87:LEU:HB3   | 2.03                     | 0.41              |
| 48:BP:114:ILE:HD12 | 48:BP:114:ILE:C    | 2.40                     | 0.41              |
| 35:BA:598:G:C5'    | 48:BP:15:ARG:HB2   | 2.40                     | 0.41              |
| 35:BA:806:C:P      | 48:BP:39:LYS:HD3   | 2.60                     | 0.41              |
| 48:BP:7:ARG:CB     | 48:BP:8:PRO:CD     | 2.94                     | 0.41              |
| 35:BA:2820:A:O4'   | 50:BR:5:LYS:HG3    | 2.20                     | 0.41              |
| 52:BT:91:ARG:HG2   | 52:BT:116:ALA:HA   | 2.02                     | 0.41              |
| 53:BU:75:ASN:ND2   | 53:BU:77:SER:OG    | 2.53                     | 0.41              |
| 53:BU:88:ILE:O     | 53:BU:90:VAL:N     | 2.50                     | 0.41              |
| 55:BW:11:ARG:O     | 55:BW:11:ARG:HD3   | 2.20                     | 0.41              |
| 57:BY:10:GLY:C     | 57:BY:27:VAL:HG13  | 2.41                     | 0.41              |
| 58:BZ:119:GLU:HG3  | 58:BZ:119:GLU:O    | 2.20                     | 0.41              |
| 58:BZ:143:GLY:O    | 58:BZ:144:LEU:HD13 | 2.20                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1169:A:H2'    | 1:CA:1170:A:C8     | 2.56                     | 0.41              |
| 1:CA:1194:U:H2'    | 1:CA:1195:C:C6     | 2.56                     | 0.41              |
| 1:CA:1269:A:H5'    | 21:CU:18:TYR:O     | 2.21                     | 0.41              |
| 1:CA:1332:A:H2'    | 1:CA:1333:A:H8     | 1.85                     | 0.41              |
| 1:CA:1442(A):G:N2  | 52:DT:119:LYS:HA   | 2.36                     | 0.41              |
| 1:CA:815:A:N6      | 1:CA:1509:C:H1'    | 2.36                     | 0.41              |
| 1:CA:154:C:H2'     | 1:CA:155:C:C6      | 2.56                     | 0.41              |
| 1:CA:334:C:H2'     | 1:CA:335:C:C6      | 2.56                     | 0.41              |
| 1:CA:542:G:H5'     | 4:CD:41:GLY:HA3    | 2.01                     | 0.41              |
| 1:CA:602:A:H2'     | 1:CA:603:U:C6      | 2.56                     | 0.41              |
| 1:CA:610:G:H2'     | 1:CA:610:G:N3      | 2.35                     | 0.41              |
| 1:CA:67:C:H2'      | 1:CA:68:G:H8       | 1.84                     | 0.41              |
| 1:CA:824:C:H2'     | 1:CA:825:G:C8      | 2.54                     | 0.41              |
| 2:CB:214:ILE:O     | 2:CB:218:ALA:HB2   | 2.20                     | 0.41              |
| 2:CB:28:PHE:CE1    | 2:CB:31:TYR:HB2    | 2.55                     | 0.41              |
| 1:CA:532:A:H61     | 3:CC:193:TYR:HB3   | 1.84                     | 0.41              |
| 4:CD:129:ASN:H     | 4:CD:129:ASN:HD22  | 1.69                     | 0.41              |
| 5:CE:76:ILE:HG22   | 5:CE:118:ILE:HD13  | 2.03                     | 0.41              |
| 5:CE:131:ILE:O     | 5:CE:134:ALA:HB3   | 2.21                     | 0.41              |
| 5:CE:149:GLU:O     | 5:CE:153:LYS:HE2   | 2.21                     | 0.41              |
| 5:CE:73:ASN:HD22   | 5:CE:73:ASN:N      | 2.16                     | 0.41              |
| 9:CI:114:TYR:N     | 9:CI:114:TYR:CD2   | 2.89                     | 0.41              |
| 10:CJ:35:SER:O     | 10:CJ:36:GLY:O     | 2.38                     | 0.41              |
| 10:CJ:81:THR:OG1   | 10:CJ:82:ILE:N     | 2.54                     | 0.41              |
| 13:CM:19:LEU:HA    | 13:CM:22:ILE:HD13  | 2.01                     | 0.41              |
| 13:CM:16:ASP:HB3   | 13:CM:41:PRO:HB3   | 2.03                     | 0.41              |
| 20:CT:18:GLN:O     | 20:CT:19:SER:C     | 2.59                     | 0.41              |
| 24:CY:298:VAL:HG22 | 24:CY:299:VAL:H    | 1.85                     | 0.41              |
| 24:CY:358:MET:HE3  | 24:CY:363:ARG:HG2  | 2.01                     | 0.41              |
| 24:CY:413:ILE:CG2  | 24:CY:413:ILE:O    | 2.68                     | 0.41              |
| 24:CY:478:LYS:HA   | 24:CY:479:PRO:HD3  | 1.75                     | 0.41              |
| 24:CY:510:VAL:HG13 | 24:CY:567:LEU:HD13 | 2.02                     | 0.41              |
| 24:CY:629:GLY:HA3  | 24:CY:647:VAL:HG12 | 2.03                     | 0.41              |
| 26:D1:49:VAL:O     | 26:D1:59:THR:HA    | 2.21                     | 0.41              |
| 27:D2:63:VAL:HG12  | 27:D2:64:LEU:N     | 2.36                     | 0.41              |
| 30:D5:29:THR:O     | 30:D5:42:PRO:HD2   | 2.21                     | 0.41              |
| 35:DA:118:A:H5'    | 35:DA:119:A:H8     | 1.85                     | 0.41              |
| 35:DA:1360:A:H5'   | 35:DA:1361:G:OP2   | 2.20                     | 0.41              |
| 35:DA:1645:G:OP1   | 35:DA:1646:C:H5'   | 2.21                     | 0.41              |
| 35:DA:1765:C:H2'   | 35:DA:1766:U:H6    | 1.86                     | 0.41              |
| 35:DA:1786:A:H2    | 35:DA:2606:C:H1'   | 1.86                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DA:18:C:O2'     | 53:DU:23:GLY:HA2   | 2.20                     | 0.41              |
| 35:DA:1960:A:H8    | 35:DA:1960:A:H5''  | 1.85                     | 0.41              |
| 35:DA:2015:A:H2'   | 35:DA:2016:U:O4'   | 2.21                     | 0.41              |
| 35:DA:2197:U:H1'   | 35:DA:2198:A:C8    | 2.55                     | 0.41              |
| 35:DA:2468:G:N2    | 35:DA:2481:G:O2'   | 2.54                     | 0.41              |
| 35:DA:2575:C:OP1   | 39:DE:144:ARG:HG3  | 2.21                     | 0.41              |
| 35:DA:2615:U:H2'   | 35:DA:2616:C:H6    | 1.85                     | 0.41              |
| 35:DA:2689:U:H4'   | 35:DA:2690:C:OP2   | 2.21                     | 0.41              |
| 35:DA:2720:U:C2    | 35:DA:2721:A:C8    | 3.09                     | 0.41              |
| 35:DA:611:C:H2'    | 35:DA:612:C:C6     | 2.55                     | 0.41              |
| 35:DA:893:C:H2'    | 35:DA:894:C:C6     | 2.55                     | 0.41              |
| 35:DA:902:C:H2'    | 35:DA:903:C:H6     | 1.86                     | 0.41              |
| 36:DB:29:A:C2      | 36:DB:56:G:C2      | 3.09                     | 0.41              |
| 37:DC:19:LYS:HG2   | 37:DC:20:VAL:N     | 2.36                     | 0.41              |
| 38:DD:205:VAL:HG12 | 38:DD:205:VAL:O    | 2.21                     | 0.41              |
| 39:DE:161:GLY:O    | 39:DE:162:ALA:C    | 2.59                     | 0.41              |
| 40:DF:152:GLU:OE1  | 40:DF:191:ARG:HD2  | 2.20                     | 0.41              |
| 40:DF:168:ARG:HG2  | 40:DF:175:THR:HG21 | 2.02                     | 0.41              |
| 40:DF:17:ARG:HG3   | 40:DF:17:ARG:NH1   | 2.35                     | 0.41              |
| 41:DG:141:PHE:O    | 41:DG:144:ILE:HG22 | 2.20                     | 0.41              |
| 41:DG:73:ALA:H     | 41:DG:87:PRO:HG2   | 1.86                     | 0.41              |
| 42:DH:106:THR:HG22 | 42:DH:112:PRO:HB3  | 2.01                     | 0.41              |
| 46:DN:3:THR:CG2    | 46:DN:4:TYR:N      | 2.80                     | 0.41              |
| 47:DO:104:ARG:HE   | 52:DT:33:LYS:CE    | 2.25                     | 0.41              |
| 48:DP:6:LEU:HG     | 48:DP:7:ARG:H      | 1.84                     | 0.41              |
| 49:DQ:34:LEU:HB2   | 49:DQ:118:LEU:HD22 | 2.03                     | 0.41              |
| 49:DQ:36:ALA:HA    | 49:DQ:129:THR:HG22 | 2.03                     | 0.41              |
| 35:DA:2838:G:C1'   | 50:DR:45:ARG:HH11  | 2.33                     | 0.41              |
| 51:DS:49:VAL:CG1   | 51:DS:50:SER:H     | 2.26                     | 0.41              |
| 53:DU:92:ARG:CZ    | 54:DV:11:GLN:H     | 2.33                     | 0.41              |
| 57:DY:28:LYS:HB2   | 57:DY:28:LYS:HE3   | 1.91                     | 0.41              |
| 58:DZ:100:VAL:CG2  | 58:DZ:126:VAL:HG21 | 2.51                     | 0.41              |
| 1:AA:1347:G:H2'    | 1:AA:1373:G:H1     | 1.85                     | 0.41              |
| 1:AA:143:A:N1      | 1:AA:220:G:O6      | 2.54                     | 0.41              |
| 1:AA:282:A:H3'     | 1:AA:283:C:C6      | 2.56                     | 0.41              |
| 1:AA:341:C:O2      | 1:AA:349:A:C2      | 2.73                     | 0.41              |
| 1:AA:652:U:C2      | 1:AA:752:G:N2      | 2.89                     | 0.41              |
| 1:AA:676:A:H1'     | 11:AK:115:PRO:HB3  | 2.03                     | 0.41              |
| 1:AA:956:U:C5      | 1:AA:957:U:C5      | 3.08                     | 0.41              |
| 4:AD:140:VAL:HG12  | 4:AD:141:ARG:O     | 2.20                     | 0.41              |
| 5:AE:145:LYS:O     | 5:AE:149:GLU:HG2   | 2.20                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:AE:34:VAL:O      | 5:AE:34:VAL:HG13   | 2.21                     | 0.41              |
| 7:AG:99:LEU:HD22   | 7:AG:103:TRP:CZ2   | 2.56                     | 0.41              |
| 7:AG:103:TRP:O     | 7:AG:104:LEU:C     | 2.58                     | 0.41              |
| 8:AH:119:LEU:HB3   | 8:AH:123:GLU:HB3   | 2.01                     | 0.41              |
| 9:AI:114:TYR:N     | 9:AI:114:TYR:CD2   | 2.88                     | 0.41              |
| 9:AI:84:ALA:C      | 9:AI:86:VAL:N      | 2.74                     | 0.41              |
| 9:AI:9:ARG:HB3     | 9:AI:104:ARG:HH12  | 1.85                     | 0.41              |
| 10:AJ:22:LYS:C     | 10:AJ:24:VAL:H     | 2.23                     | 0.41              |
| 12:AL:117:ARG:HH22 | 12:AL:124:LYS:HB2  | 1.84                     | 0.41              |
| 14:AN:12:ARG:NH1   | 14:AN:12:ARG:CB    | 2.84                     | 0.41              |
| 17:AQ:51:TYR:CE1   | 17:AQ:73:VAL:HG11  | 2.56                     | 0.41              |
| 18:AR:66:LEU:HG    | 18:AR:70:ILE:HD11  | 2.01                     | 0.41              |
| 24:AY:162:VAL:HG21 | 24:AY:255:ILE:CD1  | 2.51                     | 0.41              |
| 24:AY:514:VAL:HG21 | 24:AY:593:ALA:HB3  | 1.98                     | 0.41              |
| 24:AY:489:LYS:HG3  | 24:AY:597:GLY:HA2  | 2.03                     | 0.41              |
| 25:B0:12:ASN:C     | 25:B0:14:ARG:H     | 2.22                     | 0.41              |
| 26:B1:27:GLU:O     | 26:B1:28:GLY:C     | 2.58                     | 0.41              |
| 27:B2:8:LYS:O      | 27:B2:9:GLN:C      | 2.58                     | 0.41              |
| 29:B4:26:SER:OG    | 29:B4:27:THR:N     | 2.51                     | 0.41              |
| 35:BA:1651:G:C2    | 35:BA:2007:C:C2    | 3.09                     | 0.41              |
| 35:BA:2009:G:O2'   | 35:BA:2010:G:H5'   | 2.20                     | 0.41              |
| 35:BA:2283:C:H2'   | 35:BA:2284:C:O4'   | 2.21                     | 0.41              |
| 35:BA:2068:U:C4    | 35:BA:2430:A:H2    | 2.38                     | 0.41              |
| 35:BA:2584:U:O5'   | 35:BA:2584:U:O2    | 2.39                     | 0.41              |
| 35:BA:2706:G:N3    | 35:BA:2706:G:H2'   | 2.35                     | 0.41              |
| 35:BA:271(P):C:H2' | 35:BA:271(Q):G:O4' | 2.19                     | 0.41              |
| 35:BA:398:G:H2'    | 35:BA:399:G:C8     | 2.56                     | 0.41              |
| 35:BA:418:G:H2'    | 35:BA:419:C:H6     | 1.85                     | 0.41              |
| 35:BA:592:G:N2     | 35:BA:593:G:H1'    | 2.36                     | 0.41              |
| 35:BA:626:U:N3     | 48:BP:105:LEU:HG   | 2.35                     | 0.41              |
| 35:BA:883:G:N2     | 35:BA:894:C:C2     | 2.89                     | 0.41              |
| 35:BA:967:C:O2'    | 35:BA:968:G:H5'    | 2.20                     | 0.41              |
| 35:BA:996:A:O3'    | 53:BU:92:ARG:CG    | 2.69                     | 0.41              |
| 36:BB:36:C:H2'     | 36:BB:37:C:C6      | 2.56                     | 0.41              |
| 38:BD:14:ARG:HG3   | 38:BD:15:PHE:H     | 1.85                     | 0.41              |
| 38:BD:3:VAL:HG12   | 38:BD:17:THR:HB    | 2.03                     | 0.41              |
| 38:BD:205:VAL:HG12 | 38:BD:205:VAL:O    | 2.20                     | 0.41              |
| 38:BD:7:LYS:HB3    | 38:BD:8:PRO:HD2    | 2.03                     | 0.41              |
| 39:BE:120:TRP:CE3  | 39:BE:155:LYS:HE3  | 2.56                     | 0.41              |
| 39:BE:81:ILE:O     | 39:BE:82:ARG:C     | 2.59                     | 0.41              |
| 40:BF:187:VAL:CG1  | 48:BP:7:ARG:HH22   | 2.34                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:BG:97:ASP:O     | 41:BG:101:ILE:CG1  | 2.68                     | 0.41              |
| 41:BG:31:VAL:O     | 41:BG:33:ARG:HD3   | 2.21                     | 0.41              |
| 46:BN:2:LYS:HE2    | 53:BU:95:LEU:HD21  | 2.03                     | 0.41              |
| 48:BP:114:ILE:HG13 | 48:BP:130:PHE:HD1  | 1.85                     | 0.41              |
| 48:BP:33:ARG:O     | 48:BP:34:GLY:O     | 2.38                     | 0.41              |
| 48:BP:47:ASP:HB3   | 48:BP:48:PRO:C     | 2.41                     | 0.41              |
| 49:BQ:110:THR:HG23 | 49:BQ:113:GLN:HG3  | 2.02                     | 0.41              |
| 50:BR:28:LEU:HD23  | 50:BR:29:LEU:HD12  | 2.02                     | 0.41              |
| 52:BT:20:PRO:O     | 52:BT:22:PHE:HD2   | 2.03                     | 0.41              |
| 53:BU:50:ARG:O     | 53:BU:52:ARG:N     | 2.53                     | 0.41              |
| 53:BU:76:TYR:O     | 53:BU:79:PHE:HB3   | 2.20                     | 0.41              |
| 54:BV:38:LEU:C     | 54:BV:39:LEU:HD22  | 2.41                     | 0.41              |
| 55:BW:80:PRO:O     | 55:BW:100:THR:CG2  | 2.69                     | 0.41              |
| 35:BA:329:G:H22    | 57:BY:19:LYS:HE3   | 1.86                     | 0.41              |
| 58:BZ:122:ARG:O    | 58:BZ:123:ASP:OD1  | 2.38                     | 0.41              |
| 58:BZ:150:LEU:H    | 58:BZ:150:LEU:HD23 | 1.82                     | 0.41              |
| 1:CA:1047:G:O2'    | 1:CA:1048:G:H5'    | 2.21                     | 0.41              |
| 1:CA:1053:G:N7     | 1:CA:1200:C:C5'    | 2.76                     | 0.41              |
| 1:CA:1055:A:O5'    | 1:CA:1055:A:H8     | 2.02                     | 0.41              |
| 1:CA:1378:C:C5     | 1:CA:1379:G:C8     | 3.09                     | 0.41              |
| 1:CA:32:A:H3'      | 1:CA:33:A:H8       | 1.85                     | 0.41              |
| 1:CA:398:C:O2'     | 1:CA:399:G:H5'     | 2.21                     | 0.41              |
| 1:CA:894:G:H2'     | 1:CA:895:G:O4'     | 2.21                     | 0.41              |
| 1:CA:976:G:H5'     | 1:CA:1358:U:O2'    | 2.20                     | 0.41              |
| 5:CE:7:GLU:HG2     | 5:CE:112:LEU:HD21  | 2.02                     | 0.41              |
| 10:CJ:18:ALA:C     | 10:CJ:20:ALA:N     | 2.72                     | 0.41              |
| 13:CM:99:ARG:O     | 13:CM:100:GLY:C    | 2.58                     | 0.41              |
| 15:CO:57:LEU:N     | 15:CO:57:LEU:HD23  | 2.36                     | 0.41              |
| 17:CQ:88:TYR:O     | 17:CQ:91:ARG:N     | 2.54                     | 0.41              |
| 21:CU:24:ARG:HG2   | 21:CU:24:ARG:HH11  | 1.85                     | 0.41              |
| 22:CW:3:C:H2'      | 22:CW:4:G:H5''     | 2.01                     | 0.41              |
| 24:CY:315:LYS:C    | 24:CY:316:ILE:HD13 | 2.41                     | 0.41              |
| 24:CY:443:HIS:HB3  | 24:CY:446:THR:HG23 | 2.02                     | 0.41              |
| 24:CY:490:PRO:HG3  | 24:CY:516:PRO:HD2  | 2.02                     | 0.41              |
| 24:CY:631:ILE:HG21 | 35:DA:1067:A:N9    | 2.35                     | 0.41              |
| 25:D0:60:PHE:CD1   | 25:D0:60:PHE:C     | 2.94                     | 0.41              |
| 26:D1:67:ILE:HB    | 26:D1:68:PRO:CD    | 2.51                     | 0.41              |
| 27:D2:5:GLU:O      | 27:D2:9:GLN:HG3    | 2.20                     | 0.41              |
| 28:D3:22:ALA:CA    | 28:D3:46:ASN:HD22  | 2.34                     | 0.41              |
| 29:D4:9:LEU:HD12   | 29:D4:10:VAL:H     | 1.86                     | 0.41              |
| 30:D5:42:PRO:O     | 30:D5:43:HIS:HB2   | 2.21                     | 0.41              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:D6:53:LYS:CG    | 31:D6:54:ILE:H     | 2.33                     | 0.41              |
| 31:D6:5:VAL:HG22   | 35:DA:2283:C:OP1   | 2.21                     | 0.41              |
| 35:DA:1058:G:N2    | 44:DK:126:MET:HE3  | 2.35                     | 0.41              |
| 35:DA:1064:C:N4    | 35:DA:1074:G:H1    | 2.19                     | 0.41              |
| 35:DA:1131:G:OP1   | 46:DN:80:GLY:N     | 2.49                     | 0.41              |
| 35:DA:1214:A:H2'   | 35:DA:1215:G:O4'   | 2.21                     | 0.41              |
| 35:DA:1841:U:H2'   | 35:DA:1842:G:C8    | 2.55                     | 0.41              |
| 35:DA:185:U:H2'    | 35:DA:186:G:C8     | 2.56                     | 0.41              |
| 35:DA:212:G:O2'    | 35:DA:213:A:H5'    | 2.20                     | 0.41              |
| 35:DA:2318:G:C2'   | 35:DA:2319:G:OP1   | 2.69                     | 0.41              |
| 35:DA:2412:A:N6    | 35:DA:2413:G:C2    | 2.89                     | 0.41              |
| 35:DA:2563:U:H2'   | 35:DA:2565:A:OP2   | 2.21                     | 0.41              |
| 35:DA:803:U:HO2'   | 35:DA:804:A:H5'    | 1.84                     | 0.41              |
| 35:DA:973:A:O4'    | 35:DA:1188:U:C6    | 2.74                     | 0.41              |
| 36:DB:21:G:O2'     | 36:DB:22:U:P       | 2.78                     | 0.41              |
| 37:DC:84:ILE:HG23  | 37:DC:95:VAL:HG12  | 2.03                     | 0.41              |
| 38:DD:125:ILE:O    | 38:DD:126:GLN:HB3  | 2.20                     | 0.41              |
| 39:DE:1:MET:O      | 39:DE:2:LYS:C      | 2.58                     | 0.41              |
| 39:DE:46:ALA:HA    | 39:DE:82:ARG:O     | 2.21                     | 0.41              |
| 39:DE:82:ARG:O     | 39:DE:83:ASP:C     | 2.57                     | 0.41              |
| 40:DF:179:GLU:O    | 40:DF:181:LEU:N    | 2.54                     | 0.41              |
| 41:DG:53:LEU:HD12  | 41:DG:56:ALA:CB    | 2.50                     | 0.41              |
| 22:CV:56:C:O2      | 41:DG:83:ARG:HG2   | 2.21                     | 0.41              |
| 42:DH:105:LEU:CD2  | 42:DH:105:LEU:N    | 2.84                     | 0.41              |
| 44:DK:3:LYS:HE3    | 44:DK:29:GLN:HB3   | 2.02                     | 0.41              |
| 46:DN:97:ARG:HB3   | 46:DN:101:HIS:HD2  | 1.86                     | 0.41              |
| 48:DP:100:LEU:CD2  | 48:DP:100:LEU:N    | 2.84                     | 0.41              |
| 48:DP:114:ILE:C    | 48:DP:114:ILE:HD12 | 2.40                     | 0.41              |
| 48:DP:114:ILE:HG13 | 48:DP:130:PHE:HD1  | 1.85                     | 0.41              |
| 50:DR:13:HIS:HA    | 50:DR:17:ARG:NH2   | 2.35                     | 0.41              |
| 51:DS:70:GLY:C     | 51:DS:101:LEU:CD2  | 2.88                     | 0.41              |
| 35:DA:2376:A:N6    | 51:DS:92:TYR:HE2   | 2.19                     | 0.41              |
| 47:DO:104:ARG:NH2  | 52:DT:33:LYS:CE    | 2.80                     | 0.41              |
| 54:DV:72:VAL:HG23  | 54:DV:72:VAL:O     | 2.21                     | 0.41              |
| 35:DA:295:G:OP1    | 57:DY:2:ARG:NH2    | 2.54                     | 0.41              |
| 57:DY:28:LYS:HD2   | 57:DY:37:VAL:HG11  | 2.03                     | 0.41              |
| 58:DZ:128:VAL:CG2  | 58:DZ:132:ASN:HB2  | 2.44                     | 0.41              |
| 58:DZ:74:VAL:HG22  | 58:DZ:86:VAL:HG13  | 2.01                     | 0.41              |
| 1:AA:1014:A:H4'    | 19:AS:14:HIS:CG    | 2.55                     | 0.41              |
| 1:AA:1133:G:N3     | 1:AA:1142:G:N2     | 2.69                     | 0.41              |
| 1:AA:1090:U:H4'    | 1:AA:1170:A:C2     | 2.56                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1437:C:H2'   | 1:AA:1438:G:H8     | 1.85                     | 0.41              |
| 1:AA:814:A:H5'    | 1:AA:1511:G:H4'    | 2.02                     | 0.41              |
| 1:AA:337:C:H2'    | 1:AA:338:A:C8      | 2.56                     | 0.41              |
| 1:AA:977:A:H3'    | 1:AA:977:A:N3      | 2.34                     | 0.41              |
| 2:AB:222:ILE:HB   | 2:AB:226:ARG:NH2   | 2.31                     | 0.41              |
| 4:AD:102:ASP:HA   | 4:AD:121:VAL:HG21  | 2.02                     | 0.41              |
| 9:AI:33:PHE:O     | 9:AI:35:GLU:N      | 2.49                     | 0.41              |
| 10:AJ:6:ILE:CG2   | 10:AJ:98:ILE:HD12  | 2.41                     | 0.41              |
| 12:AL:17:LYS:CD   | 12:AL:18:VAL:HG22  | 2.47                     | 0.41              |
| 13:AM:36:LYS:HG3  | 13:AM:59:TYR:OH    | 2.21                     | 0.41              |
| 13:AM:81:LEU:H    | 13:AM:81:LEU:HD22  | 1.83                     | 0.41              |
| 14:AN:27:CYS:SG   | 14:AN:40:CYS:SG    | 3.18                     | 0.41              |
| 16:AP:32:TYR:CD2  | 16:AP:32:TYR:O     | 2.61                     | 0.41              |
| 17:AQ:21:VAL:HG21 | 17:AQ:59:ILE:HD11  | 2.03                     | 0.41              |
| 17:AQ:45:HIS:O    | 17:AQ:73:VAL:HG23  | 2.21                     | 0.41              |
| 20:AT:33:ILE:O    | 20:AT:37:SER:OG    | 2.34                     | 0.41              |
| 24:AY:111:SER:O   | 24:AY:112:GLN:C    | 2.58                     | 0.41              |
| 24:AY:25:LYS:N    | 62:AY:703:GDP:O2B  | 2.54                     | 0.41              |
| 24:AY:364:GLU:HG2 | 24:AY:366:VAL:HG13 | 2.03                     | 0.41              |
| 24:AY:447:GLY:O   | 24:AY:448:GLN:C    | 2.58                     | 0.41              |
| 24:AY:530:VAL:CG2 | 24:AY:531:GLY:N    | 2.79                     | 0.41              |
| 24:AY:138:LYS:HE2 | 62:AY:703:GDP:C4   | 2.56                     | 0.41              |
| 26:B1:84:GLY:O    | 26:B1:85:LEU:C     | 2.59                     | 0.41              |
| 27:B2:67:LYS:O    | 27:B2:69:ARG:N     | 2.53                     | 0.41              |
| 29:B4:10:VAL:CG2  | 29:B4:11:PRO:CD    | 2.99                     | 0.41              |
| 29:B4:6:HIS:C     | 29:B4:8:LYS:N      | 2.74                     | 0.41              |
| 31:B6:20:ASN:ND2  | 31:B6:44:ARG:HH22  | 2.18                     | 0.41              |
| 35:BA:1141:U:OP1  | 46:BN:25:ARG:NH1   | 2.54                     | 0.41              |
| 35:BA:1164:G:H1   | 35:BA:1185:C:N4    | 2.19                     | 0.41              |
| 35:BA:1497:U:C2   | 35:BA:1578:U:OP1   | 2.74                     | 0.41              |
| 35:BA:1573:G:C2'  | 35:BA:1574:C:H5'   | 2.51                     | 0.41              |
| 35:BA:1697:G:H3'  | 35:BA:1698:A:C5'   | 2.47                     | 0.41              |
| 35:BA:1882:C:H2'  | 35:BA:1883:G:O4'   | 2.20                     | 0.41              |
| 35:BA:2464:C:O2'  | 35:BA:2465:C:P     | 2.78                     | 0.41              |
| 35:BA:2572:A:C5'  | 35:BA:2574:G:H4'   | 2.35                     | 0.41              |
| 35:BA:2681:C:H5   | 35:BA:2725:A:N6    | 2.18                     | 0.41              |
| 35:BA:2712:U:O4'  | 35:BA:2712:U:O2    | 2.39                     | 0.41              |
| 35:BA:2838:G:C1'  | 50:BR:45:ARG:HH11  | 2.34                     | 0.41              |
| 35:BA:464:U:H2'   | 35:BA:465:G:O4'    | 2.21                     | 0.41              |
| 35:BA:64:A:O2'    | 35:BA:65:C:H5'     | 2.20                     | 0.41              |
| 35:BA:657:U:H2'   | 35:BA:658:C:C5     | 2.55                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:192:C:O2'    | 35:BA:802:A:N3     | 2.49                     | 0.41              |
| 35:BA:861:A:C2     | 35:BA:917:A:C4     | 3.09                     | 0.41              |
| 37:BC:118:PRO:C    | 37:BC:121:MET:HG2  | 2.42                     | 0.41              |
| 37:BC:138:LEU:HD22 | 37:BC:139:PRO:CD   | 2.49                     | 0.41              |
| 38:BD:124:PRO:O    | 38:BD:129:ASN:ND2  | 2.53                     | 0.41              |
| 38:BD:138:VAL:O    | 38:BD:138:VAL:HG13 | 2.21                     | 0.41              |
| 39:BE:117:MET:HA   | 39:BE:122:PHE:N    | 2.18                     | 0.41              |
| 39:BE:26:ILE:CG2   | 39:BE:196:VAL:HG21 | 2.47                     | 0.41              |
| 40:BF:10:PRO:HG2   | 40:BF:11:VAL:N     | 2.36                     | 0.41              |
| 40:BF:110:LEU:CD1  | 40:BF:202:PHE:HE1  | 2.34                     | 0.41              |
| 41:BG:111:LEU:HD21 | 41:BG:120:LEU:HD21 | 2.02                     | 0.41              |
| 41:BG:133:LEU:C    | 41:BG:133:LEU:CD1  | 2.89                     | 0.41              |
| 46:BN:22:THR:HB    | 46:BN:25:ARG:CB    | 2.47                     | 0.41              |
| 35:BA:1996:C:OP1   | 47:BO:31:LYS:HE2   | 2.20                     | 0.41              |
| 47:BO:53:LYS:O     | 47:BO:54:GLU:O     | 2.38                     | 0.41              |
| 48:BP:31:ALA:C     | 48:BP:33:ARG:N     | 2.73                     | 0.41              |
| 50:BR:3:HIS:O      | 50:BR:4:LEU:CB     | 2.68                     | 0.41              |
| 51:BS:15:ARG:CB    | 51:BS:18:ILE:HD11  | 2.36                     | 0.41              |
| 51:BS:92:TYR:CG    | 51:BS:93:LYS:N     | 2.89                     | 0.41              |
| 55:BW:37:ARG:HG3   | 55:BW:38:TYR:CD2   | 2.55                     | 0.41              |
| 56:BX:47:PHE:CD2   | 56:BX:89:ILE:HG21  | 2.55                     | 0.41              |
| 58:BZ:103:ARG:HD2  | 58:BZ:136:PHE:CG   | 2.56                     | 0.41              |
| 58:BZ:47:VAL:O     | 58:BZ:51:ALA:HB3   | 2.20                     | 0.41              |
| 58:BZ:97:GLU:HB3   | 58:BZ:125:LEU:HD11 | 2.03                     | 0.41              |
| 1:CA:1037:C:H2'    | 1:CA:1038:C:N3     | 2.34                     | 0.41              |
| 1:CA:1134:G:H2'    | 1:CA:1135:U:H5'    | 2.03                     | 0.41              |
| 1:CA:1392:G:N2     | 1:CA:1502:A:H8     | 2.19                     | 0.41              |
| 1:CA:1452:C:O4'    | 1:CA:1452:C:OP1    | 2.39                     | 0.41              |
| 1:CA:176:C:C2      | 1:CA:177:C:C5      | 3.08                     | 0.41              |
| 1:CA:261:U:N3      | 1:CA:264:U:OP2     | 2.42                     | 0.41              |
| 2:CB:158:LEU:HA    | 2:CB:159:PRO:HD3   | 1.93                     | 0.41              |
| 2:CB:194:PRO:O     | 2:CB:195:ASP:C     | 2.60                     | 0.41              |
| 3:CC:59:ARG:HG3    | 3:CC:64:VAL:HA     | 2.01                     | 0.41              |
| 4:CD:133:VAL:HG12  | 4:CD:134:ASP:N     | 2.35                     | 0.41              |
| 10:CJ:31:GLY:O     | 10:CJ:32:ALA:C     | 2.58                     | 0.41              |
| 14:CN:29:ARG:HH11  | 14:CN:29:ARG:CG    | 2.31                     | 0.41              |
| 14:CN:5:ALA:O      | 14:CN:8:GLU:HB2    | 2.21                     | 0.41              |
| 14:CN:9:LYS:HE3    | 14:CN:9:LYS:HB2    | 1.91                     | 0.41              |
| 19:CS:20:LEU:HD23  | 19:CS:20:LEU:HA    | 1.83                     | 0.41              |
| 22:CW:46:G:O2'     | 22:CW:47:G:H5'     | 2.20                     | 0.41              |
| 24:CY:15:ILE:HD13  | 24:CY:105:ILE:CD1  | 2.50                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:CY:20:HIS:O     | 24:CY:23:ALA:HB2   | 2.20                     | 0.41              |
| 24:CY:606:MET:SD   | 24:CY:673:PHE:HA   | 2.60                     | 0.41              |
| 29:D4:10:VAL:CG1   | 29:D4:27:THR:HA    | 2.51                     | 0.41              |
| 29:D4:27:THR:O     | 29:D4:28:LYS:CB    | 2.69                     | 0.41              |
| 29:D4:48:ARG:O     | 29:D4:49:PHE:HD1   | 2.01                     | 0.41              |
| 30:D5:44:THR:O     | 30:D5:51:TYR:CE1   | 2.70                     | 0.41              |
| 35:DA:82:G:N1      | 35:DA:103:A:OP2    | 2.53                     | 0.41              |
| 35:DA:1196:C:O2'   | 35:DA:1197:G:H5'   | 2.21                     | 0.41              |
| 35:DA:128:C:O2'    | 35:DA:129:C:P      | 2.79                     | 0.41              |
| 35:DA:1453:U:H2'   | 35:DA:1455:G:C8    | 2.56                     | 0.41              |
| 35:DA:1472:A:H2'   | 35:DA:1473:G:H8    | 1.85                     | 0.41              |
| 35:DA:1528(A):A:C8 | 35:DA:1529:G:C8    | 3.09                     | 0.41              |
| 35:DA:1539:G:N1    | 35:DA:1540:U:O2    | 2.54                     | 0.41              |
| 35:DA:1664:A:OP1   | 35:DA:1665:A:OP2   | 2.39                     | 0.41              |
| 35:DA:2020:A:C6    | 35:DA:2022:U:C2    | 3.08                     | 0.41              |
| 35:DA:2370:G:H2'   | 35:DA:2371:G:O4'   | 2.21                     | 0.41              |
| 35:DA:2534:A:H2'   | 35:DA:2535:G:O5'   | 2.20                     | 0.41              |
| 30:D5:3:LYS:NZ     | 35:DA:2613:U:O2'   | 2.49                     | 0.41              |
| 35:DA:2825:C:H2'   | 35:DA:2826:A:O4'   | 2.21                     | 0.41              |
| 35:DA:361:G:N2     | 35:DA:362:U:H1'    | 2.35                     | 0.41              |
| 35:DA:483:A:H3'    | 35:DA:484:C:C6     | 2.56                     | 0.41              |
| 35:DA:606:U:C2'    | 35:DA:606:U:O2     | 2.65                     | 0.41              |
| 35:DA:820:A:N3     | 35:DA:943:U:O2'    | 2.47                     | 0.41              |
| 36:DB:5:C:O2'      | 36:DB:6:C:H5'      | 2.21                     | 0.41              |
| 37:DC:134:PRO:HB2  | 37:DC:135:ARG:HD2  | 2.03                     | 0.41              |
| 38:DD:266:SER:C    | 38:DD:267:SER:O    | 2.59                     | 0.41              |
| 39:DE:137:HIS:CB   | 39:DE:138:PRO:HD2  | 2.51                     | 0.41              |
| 39:DE:59:VAL:CG2   | 39:DE:62:PRO:O     | 2.69                     | 0.41              |
| 40:DF:168:ARG:O    | 40:DF:170:LEU:N    | 2.53                     | 0.41              |
| 35:DA:1248:G:OP2   | 40:DF:92:PRO:HB3   | 2.20                     | 0.41              |
| 41:DG:77:ILE:C     | 41:DG:80:PHE:H     | 2.23                     | 0.41              |
| 42:DH:169:VAL:HG13 | 42:DH:170:ARG:H    | 1.82                     | 0.41              |
| 44:DK:121:GLU:O    | 44:DK:125:ARG:NE   | 2.53                     | 0.41              |
| 44:DK:61:ALA:O     | 44:DK:63:ARG:N     | 2.54                     | 0.41              |
| 46:DN:94:HIS:HA    | 46:DN:96:GLU:OE1   | 2.21                     | 0.41              |
| 47:DO:69:ILE:HD13  | 47:DO:77:ILE:CG2   | 2.42                     | 0.41              |
| 48:DP:56:SER:O     | 48:DP:58:THR:N     | 2.54                     | 0.41              |
| 48:DP:83:VAL:H     | 48:DP:115:LEU:HD23 | 1.83                     | 0.41              |
| 52:DT:19:LEU:HA    | 52:DT:20:PRO:HD3   | 1.81                     | 0.41              |
| 54:DV:64:HIS:HA    | 54:DV:92:THR:HA    | 2.03                     | 0.41              |
| 1:AA:1053:G:C4     | 1:AA:1199:U:C5     | 3.08                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1250:A:C2     | 1:AA:1251:A:C4     | 3.09                     | 0.41              |
| 1:AA:1277:C:H2'    | 1:AA:1278:U:C5'    | 2.42                     | 0.41              |
| 1:AA:1284:C:O5'    | 1:AA:1284:C:H6     | 2.03                     | 0.41              |
| 1:AA:1442(B):A:N3  | 1:AA:1442(B):A:H2' | 2.36                     | 0.41              |
| 1:AA:201:C:C3'     | 1:AA:202:U:H5''    | 2.51                     | 0.41              |
| 1:AA:439:A:H2'     | 1:AA:441:A:C5'     | 2.51                     | 0.41              |
| 1:AA:470:C:H2'     | 1:AA:471:G:OP1     | 2.21                     | 0.41              |
| 1:AA:794:A:O2'     | 1:AA:795:C:H5'     | 2.21                     | 0.41              |
| 3:AC:53:ALA:HB2    | 3:AC:115:LEU:HG    | 2.02                     | 0.41              |
| 3:AC:136:GLN:HG3   | 3:AC:139:GLN:CB    | 2.47                     | 0.41              |
| 3:AC:141:VAL:O     | 3:AC:144:SER:N     | 2.53                     | 0.41              |
| 3:AC:30:ARG:HD2    | 14:AN:38:GLY:HA3   | 2.03                     | 0.41              |
| 5:AE:59:GLY:O      | 5:AE:62:ALA:HB3    | 2.21                     | 0.41              |
| 7:AG:138:LYS:HE3   | 7:AG:142:GLU:OE1   | 2.21                     | 0.41              |
| 7:AG:137:LYS:HE2   | 7:AG:141:VAL:HG23  | 2.03                     | 0.41              |
| 9:AI:77:ILE:O      | 9:AI:78:LYS:C      | 2.59                     | 0.41              |
| 10:AJ:4:ILE:HD12   | 10:AJ:4:ILE:H      | 1.81                     | 0.41              |
| 11:AK:33:THR:HB    | 11:AK:38:ASN:C     | 2.41                     | 0.41              |
| 12:AL:47:LYS:CD    | 12:AL:48:PRO:HD3   | 2.49                     | 0.41              |
| 15:AO:55:GLY:O     | 15:AO:56:LEU:C     | 2.59                     | 0.41              |
| 15:AO:74:ASP:OD1   | 15:AO:76:GLU:HB3   | 2.21                     | 0.41              |
| 1:AA:277:C:H5'     | 17:AQ:68:ARG:NH1   | 2.36                     | 0.41              |
| 20:AT:75:ASN:O     | 20:AT:76:ALA:C     | 2.59                     | 0.41              |
| 23:AX:13:A:C3'     | 23:AX:14:A:C5'     | 2.78                     | 0.41              |
| 24:AY:117:GLN:O    | 24:AY:118:SER:C    | 2.58                     | 0.41              |
| 24:AY:120:THR:O    | 24:AY:124:GLN:CD   | 2.59                     | 0.41              |
| 24:AY:188:TYR:OH   | 24:AY:271:LEU:HD11 | 2.21                     | 0.41              |
| 24:AY:485:GLU:CB   | 24:AY:560:VAL:HG22 | 2.48                     | 0.41              |
| 24:AY:621:ILE:HG23 | 24:AY:631:ILE:HG12 | 2.02                     | 0.41              |
| 24:AY:138:LYS:HE2  | 62:AY:703:GDP:N9   | 2.36                     | 0.41              |
| 28:B3:35:ARG:CD    | 28:B3:37:LEU:HD21  | 2.51                     | 0.41              |
| 29:B4:10:VAL:CG1   | 29:B4:27:THR:HA    | 2.51                     | 0.41              |
| 30:B5:2:ALA:N      | 35:BA:2015:A:C1'   | 2.84                     | 0.41              |
| 35:BA:1221(A):C:C2 | 35:BA:1229:G:N2    | 2.89                     | 0.41              |
| 35:BA:1657:C:H2'   | 35:BA:1658:C:C6    | 2.55                     | 0.41              |
| 35:BA:1803:A:C8    | 35:BA:1804:C:C5    | 3.09                     | 0.41              |
| 35:BA:20:C:H2'     | 35:BA:21:A:C8      | 2.54                     | 0.41              |
| 35:BA:2318:G:C2'   | 35:BA:2319:G:OP1   | 2.69                     | 0.41              |
| 35:BA:2534:A:H2'   | 35:BA:2535:G:O5'   | 2.21                     | 0.41              |
| 35:BA:2880:C:H6    | 35:BA:2880:C:O5'   | 2.04                     | 0.41              |
| 35:BA:688:U:H2'    | 35:BA:689:A:H8     | 1.86                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:464:U:C4     | 35:BA:788:A:N7     | 2.89                     | 0.41              |
| 35:BA:954:G:O2'    | 35:BA:955:C:H5'    | 2.21                     | 0.41              |
| 36:BB:9:G:C6       | 36:BB:113:G:C6     | 3.09                     | 0.41              |
| 38:BD:67:PHE:HD2   | 38:BD:67:PHE:HA    | 1.73                     | 0.41              |
| 39:BE:183:LEU:HD12 | 39:BE:183:LEU:N    | 2.34                     | 0.41              |
| 39:BE:46:ALA:HA    | 39:BE:82:ARG:O     | 2.21                     | 0.41              |
| 40:BF:181:LEU:O    | 40:BF:205:ARG:NH1  | 2.54                     | 0.41              |
| 41:BG:102:PHE:O    | 41:BG:105:LYS:N    | 2.53                     | 0.41              |
| 41:BG:56:ALA:CA    | 41:BG:59:GLU:OE1   | 2.66                     | 0.41              |
| 41:BG:77:ILE:O     | 41:BG:78:SER:C     | 2.59                     | 0.41              |
| 44:BK:55:VAL:HG13  | 44:BK:57:ILE:HD11  | 2.03                     | 0.41              |
| 44:BK:6:ALA:CB     | 44:BK:30:HIS:CE1   | 3.04                     | 0.41              |
| 46:BN:76:SER:O     | 46:BN:78:TYR:N     | 2.53                     | 0.41              |
| 46:BN:79:PRO:C     | 46:BN:81:GLY:H     | 2.24                     | 0.41              |
| 51:BS:49:VAL:CG1   | 51:BS:50:SER:N     | 2.79                     | 0.41              |
| 51:BS:87:PHE:HB2   | 51:BS:106:ARG:HH21 | 1.85                     | 0.41              |
| 52:BT:30:VAL:HG22  | 52:BT:84:GLN:O     | 2.21                     | 0.41              |
| 53:BU:21:ALA:HA    | 53:BU:24:TYR:CE1   | 2.56                     | 0.41              |
| 53:BU:46:ALA:O     | 53:BU:47:TYR:C     | 2.59                     | 0.41              |
| 54:BV:64:HIS:HA    | 54:BV:92:THR:HA    | 2.01                     | 0.41              |
| 53:BU:50:ARG:HH11  | 54:BV:70:ILE:CG2   | 2.34                     | 0.41              |
| 55:BW:70:TYR:O     | 55:BW:107:LEU:HB3  | 2.21                     | 0.41              |
| 55:BW:36:LEU:CD1   | 55:BW:47:VAL:HG12  | 2.49                     | 0.41              |
| 55:BW:6:ILE:HA     | 55:BW:103:ILE:O    | 2.20                     | 0.41              |
| 58:BZ:78:LYS:H     | 58:BZ:78:LYS:HD3   | 1.86                     | 0.41              |
| 1:CA:103:C:H2'     | 1:CA:103:C:O2      | 2.21                     | 0.41              |
| 1:CA:1074:G:O2'    | 1:CA:1075:C:H5'    | 2.20                     | 0.41              |
| 1:CA:252:U:C4      | 1:CA:253:U:O4      | 2.74                     | 0.41              |
| 1:CA:318:G:C2      | 1:CA:336:C:N3      | 2.89                     | 0.41              |
| 1:CA:323:U:H2'     | 1:CA:324:G:O4'     | 2.21                     | 0.41              |
| 1:CA:470:C:H2'     | 1:CA:471:G:OP1     | 2.21                     | 0.41              |
| 1:CA:619:U:O5'     | 1:CA:619:U:H6      | 2.04                     | 0.41              |
| 1:CA:748:C:O2'     | 1:CA:749:C:H6      | 2.04                     | 0.41              |
| 1:CA:802:A:H3'     | 1:CA:803:G:C8      | 2.56                     | 0.41              |
| 1:CA:953:G:H5'     | 1:CA:965:A:N6      | 2.28                     | 0.41              |
| 1:CA:992:U:HO2'    | 1:CA:993:G:P       | 2.44                     | 0.41              |
| 2:CB:213:LEU:O     | 2:CB:213:LEU:HD23  | 2.20                     | 0.41              |
| 3:CC:14:ILE:CG1    | 3:CC:15:THR:N      | 2.84                     | 0.41              |
| 3:CC:83:ARG:O      | 3:CC:86:VAL:N      | 2.54                     | 0.41              |
| 4:CD:18:LYS:HE2    | 4:CD:20:TYR:CE2    | 2.56                     | 0.41              |
| 4:CD:6:GLY:O       | 4:CD:7:PRO:C       | 2.59                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 4:CD:97:LEU:HA      | 4:CD:97:LEU:HD23   | 1.85                     | 0.41              |
| 5:CE:88:LYS:HB3     | 5:CE:123:LEU:O     | 2.20                     | 0.41              |
| 8:CH:36:LEU:O       | 8:CH:37:ARG:C      | 2.58                     | 0.41              |
| 9:CI:79:LEU:O       | 9:CI:82:ALA:N      | 2.54                     | 0.41              |
| 9:CI:50:LEU:HD23    | 9:CI:85:LEU:CD2    | 2.50                     | 0.41              |
| 9:CI:84:ALA:C       | 9:CI:86:VAL:N      | 2.73                     | 0.41              |
| 10:CJ:6:ILE:O       | 10:CJ:71:LEU:HD12  | 2.21                     | 0.41              |
| 11:CK:21:ILE:HG13   | 11:CK:30:VAL:CG1   | 2.51                     | 0.41              |
| 13:CM:88:ARG:HG2    | 13:CM:88:ARG:HH11  | 1.86                     | 0.41              |
| 15:CO:43:LEU:C      | 15:CO:45:VAL:N     | 2.74                     | 0.41              |
| 20:CT:33:ILE:HD11   | 20:CT:62:LEU:O     | 2.21                     | 0.41              |
| 22:CV:61:C:H2'      | 22:CV:62:C:H6      | 1.86                     | 0.41              |
| 24:CY:126:GLU:O     | 24:CY:129:LYS:N    | 2.54                     | 0.41              |
| 24:CY:151:ARG:O     | 24:CY:155:GLU:HB2  | 2.21                     | 0.41              |
| 24:CY:229:LEU:HA    | 24:CY:232:LEU:HD23 | 2.02                     | 0.41              |
| 24:CY:352:VAL:HG23  | 24:CY:377:VAL:HB   | 2.01                     | 0.41              |
| 24:CY:138:LYS:HG2   | 62:CY:703:GDP:C6   | 2.54                     | 0.41              |
| 25:D0:40:GLN:HE21   | 25:D0:43:THR:HA    | 1.77                     | 0.41              |
| 26:D1:26:ARG:HG3    | 26:D1:27:GLU:CG    | 2.43                     | 0.41              |
| 35:DA:1144:G:C6     | 35:DA:1145:C:C4    | 3.08                     | 0.41              |
| 35:DA:130:C:O3'     | 35:DA:1349:A:H1'   | 2.21                     | 0.41              |
| 35:DA:1495:A:H2'    | 35:DA:1496:A:N3    | 2.36                     | 0.41              |
| 35:DA:1820:U:H3     | 38:DD:199:ALA:HA   | 1.86                     | 0.41              |
| 35:DA:2115:G:C3'    | 35:DA:2116:G:H5''  | 2.51                     | 0.41              |
| 35:DA:2322:A:O2'    | 35:DA:2323:G:H5'   | 2.21                     | 0.41              |
| 35:DA:2617:C:H2'    | 35:DA:2618:G:H5'   | 2.02                     | 0.41              |
| 35:DA:2618:G:H2'    | 35:DA:2619:C:C6    | 2.55                     | 0.41              |
| 35:DA:2751:G:N2     | 35:DA:2751:G:OP1   | 2.54                     | 0.41              |
| 35:DA:2820:A:O4'    | 50:DR:5:LYS:HG3    | 2.20                     | 0.41              |
| 35:DA:437:G:H2'     | 35:DA:438:G:C8     | 2.56                     | 0.41              |
| 35:DA:614(B):G:H5'' | 35:DA:614(C):A:OP1 | 2.21                     | 0.41              |
| 35:DA:677:A:O2'     | 35:DA:678:C:H5'    | 2.21                     | 0.41              |
| 35:DA:78:A:H2'      | 35:DA:79:G:H8      | 1.85                     | 0.41              |
| 35:DA:813:U:C2      | 35:DA:814:C:C5     | 3.09                     | 0.41              |
| 37:DC:117:THR:O     | 37:DC:120:VAL:HG22 | 2.21                     | 0.41              |
| 35:DA:2128:C:OP1    | 37:DC:37:LYS:HG3   | 2.21                     | 0.41              |
| 37:DC:46:ALA:O      | 37:DC:48:LEU:HD12  | 2.21                     | 0.41              |
| 35:DA:2786:U:O2'    | 39:DE:62:PRO:HA    | 2.20                     | 0.41              |
| 40:DF:103:LYS:HA    | 40:DF:106:ARG:CG   | 2.51                     | 0.41              |
| 40:DF:133:ASN:N     | 40:DF:162:LEU:HD23 | 2.35                     | 0.41              |
| 41:DG:114:ILE:O     | 41:DG:115:ARG:HB2  | 2.20                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:DG:34:LEU:HD13  | 41:DG:99:MET:CE    | 2.51                     | 0.41              |
| 41:DG:49:ASP:O     | 41:DG:50:ALA:HB3   | 2.20                     | 0.41              |
| 42:DH:128:PRO:HG2  | 42:DH:129:THR:HG23 | 2.03                     | 0.41              |
| 42:DH:61:HIS:O     | 42:DH:62:LYS:C     | 2.57                     | 0.41              |
| 42:DH:76:VAL:C     | 42:DH:78:GLY:N     | 2.74                     | 0.41              |
| 44:DK:48:MET:HB2   | 44:DK:49:GLY:H     | 1.70                     | 0.41              |
| 46:DN:120:LEU:HD13 | 46:DN:121:LYS:N    | 2.36                     | 0.41              |
| 46:DN:79:PRO:C     | 46:DN:81:GLY:H     | 2.24                     | 0.41              |
| 48:DP:106:LEU:HD12 | 48:DP:106:LEU:N    | 2.36                     | 0.41              |
| 49:DQ:55:VAL:CG1   | 49:DQ:56:ARG:H     | 2.29                     | 0.41              |
| 50:DR:38:VAL:HB    | 50:DR:39:PRO:CD    | 2.39                     | 0.41              |
| 51:DS:101:LEU:O    | 51:DS:102:ALA:O    | 2.39                     | 0.41              |
| 51:DS:74:ALA:CB    | 51:DS:103:GLU:HB2  | 2.46                     | 0.41              |
| 53:DU:50:ARG:O     | 53:DU:52:ARG:N     | 2.53                     | 0.41              |
| 55:DW:10:VAL:HG21  | 55:DW:103:ILE:HG13 | 2.03                     | 0.41              |
| 57:DY:77:PRO:HB2   | 57:DY:99:CYS:SG    | 2.61                     | 0.41              |
| 57:DY:87:LYS:O     | 57:DY:88:LYS:HB2   | 2.20                     | 0.41              |
| 58:DZ:28:MET:O     | 58:DZ:34:ASN:HB2   | 2.21                     | 0.41              |
| 1:AA:1037:C:H2'    | 1:AA:1038:C:N3     | 2.35                     | 0.41              |
| 1:AA:1255:G:H2'    | 1:AA:1279:A:H62    | 1.86                     | 0.41              |
| 1:AA:1371:G:OP2    | 9:AI:11:LYS:HD2    | 2.21                     | 0.41              |
| 1:AA:32:A:C2       | 1:AA:33:A:C4       | 3.09                     | 0.41              |
| 1:AA:340:U:C2      | 1:AA:350:G:C2      | 3.09                     | 0.41              |
| 1:AA:432:A:N7      | 1:AA:433:C:C4      | 2.89                     | 0.41              |
| 1:AA:585:G:C6      | 1:AA:586:C:C4      | 3.08                     | 0.41              |
| 1:AA:619:U:H6      | 1:AA:619:U:O5'     | 2.03                     | 0.41              |
| 1:AA:953:G:H5'     | 1:AA:965:A:N6      | 2.30                     | 0.41              |
| 2:AB:121:LEU:HA    | 2:AB:124:SER:CB    | 2.51                     | 0.41              |
| 3:AC:22:TRP:CH2    | 3:AC:32:LEU:HB2    | 2.55                     | 0.41              |
| 4:AD:165:MET:HE2   | 4:AD:176:LEU:HD22  | 2.03                     | 0.41              |
| 4:AD:173:TRP:CB    | 4:AD:187:ARG:NH1   | 2.83                     | 0.41              |
| 7:AG:15:ASP:OD2    | 7:AG:16:LEU:N      | 2.54                     | 0.41              |
| 8:AH:1:MET:O       | 8:AH:2:LEU:O       | 2.39                     | 0.41              |
| 9:AI:8:GLY:HA3     | 9:AI:79:LEU:HB3    | 2.03                     | 0.41              |
| 10:AJ:39:PRO:HG2   | 10:AJ:39:PRO:O     | 2.21                     | 0.41              |
| 10:AJ:38:ILE:N     | 10:AJ:71:LEU:O     | 2.50                     | 0.41              |
| 13:AM:66:LEU:O     | 13:AM:67:GLU:O     | 2.38                     | 0.41              |
| 15:AO:80:ALA:O     | 15:AO:81:LEU:C     | 2.59                     | 0.41              |
| 18:AR:26:LEU:CD2   | 18:AR:42:ARG:NH1   | 2.84                     | 0.41              |
| 19:AS:9:VAL:HG13   | 19:AS:39:THR:HB    | 2.03                     | 0.41              |
| 20:AT:38:LYS:O     | 20:AT:39:LYS:C     | 2.58                     | 0.41              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:AY:402:ILE:H   | 24:AY:402:ILE:CD1  | 2.33                     | 0.41              |
| 24:AY:610:VAL:CG2 | 24:AY:643:ILE:HB   | 2.51                     | 0.41              |
| 24:AY:673:PHE:CD2 | 24:AY:674:ASP:N    | 2.89                     | 0.41              |
| 24:AY:83:ASP:O    | 24:AY:84:THR:OG1   | 2.32                     | 0.41              |
| 24:AY:89:ASP:HB2  | 24:AY:90:PHE:H     | 1.36                     | 0.41              |
| 27:B2:3:LEU:CD2   | 27:B2:7:ARG:HH12   | 2.14                     | 0.41              |
| 31:B6:53:LYS:CG   | 31:B6:54:ILE:H     | 2.34                     | 0.41              |
| 33:B8:50:LEU:C    | 33:B8:52:LYS:N     | 2.74                     | 0.41              |
| 35:BA:1251:C:OP2  | 53:BU:10:ARG:NE    | 2.50                     | 0.41              |
| 35:BA:1326:U:H4'  | 35:BA:2011:U:O4'   | 2.20                     | 0.41              |
| 35:BA:1491:G:N3   | 35:BA:1492:G:C8    | 2.89                     | 0.41              |
| 35:BA:1526:G:H2'  | 35:BA:1527:G:O4'   | 2.21                     | 0.41              |
| 35:BA:1529:G:C6   | 35:BA:1541:G:N1    | 2.88                     | 0.41              |
| 35:BA:1683:C:O2'  | 35:BA:1684:C:H5'   | 2.21                     | 0.41              |
| 35:BA:1721:G:C2   | 35:BA:1739:U:OP2   | 2.74                     | 0.41              |
| 35:BA:1941:C:C4   | 35:BA:1942:C:C4    | 3.09                     | 0.41              |
| 35:BA:2018:G:H21  | 53:BU:34:LYS:HZ2   | 1.68                     | 0.41              |
| 35:BA:2134:A:H1'  | 35:BA:2158:A:C2    | 2.56                     | 0.41              |
| 35:BA:239:U:H1'   | 35:BA:259:G:N2     | 2.36                     | 0.41              |
| 35:BA:1638:C:H1'  | 35:BA:2698:U:O2'   | 2.21                     | 0.41              |
| 35:BA:270:A:O2'   | 35:BA:271:A:H5'    | 2.20                     | 0.41              |
| 35:BA:705:A:C6    | 35:BA:727:A:H1'    | 2.56                     | 0.41              |
| 35:BA:733:G:C6    | 35:BA:761:A:C8     | 3.09                     | 0.41              |
| 35:BA:763:G:C4    | 35:BA:765:G:C8     | 3.09                     | 0.41              |
| 36:BB:74:U:C2'    | 36:BB:75:G:H5'     | 2.51                     | 0.41              |
| 36:BB:77:U:OP1    | 58:BZ:19:ARG:NH2   | 2.53                     | 0.41              |
| 37:BC:119:ASP:OD1 | 37:BC:120:VAL:HG13 | 2.21                     | 0.41              |
| 38:BD:126:GLN:O   | 38:BD:127:VAL:C    | 2.59                     | 0.41              |
| 39:BE:9:VAL:HG22  | 39:BE:10:GLY:H     | 1.84                     | 0.41              |
| 39:BE:128:SER:OG  | 39:BE:129:HIS:N    | 2.54                     | 0.41              |
| 39:BE:143:ASN:N   | 39:BE:143:ASN:ND2  | 2.69                     | 0.41              |
| 42:BH:12:PRO:HB2  | 42:BH:15:VAL:CG1   | 2.40                     | 0.41              |
| 42:BH:97:ARG:O    | 42:BH:97:ARG:HG2   | 2.21                     | 0.41              |
| 35:BA:1084:A:OP1  | 43:BJ:55:UNK:HA    | 2.20                     | 0.41              |
| 44:BK:8:VAL:O     | 44:BK:56:GLU:HA    | 2.21                     | 0.41              |
| 35:BA:558:G:OP1   | 46:BN:111:PRO:HD2  | 2.20                     | 0.41              |
| 48:BP:119:GLU:HA  | 48:BP:119:GLU:OE1  | 2.21                     | 0.41              |
| 49:BQ:37:LEU:HG   | 49:BQ:129:THR:HA   | 2.03                     | 0.41              |
| 1:AA:1442(B):A:C5 | 52:BT:118:ARG:NE   | 2.89                     | 0.41              |
| 52:BT:90:GLN:O    | 52:BT:92:GLY:N     | 2.53                     | 0.41              |
| 56:BX:64:LYS:HE2  | 56:BX:64:LYS:HB3   | 1.85                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 56:BX:90:GLU:O    | 56:BX:92:LEU:N    | 2.53                     | 0.41              |
| 57:BY:96:ILE:HG21 | 57:BY:99:CYS:HB3  | 2.02                     | 0.41              |
| 58:BZ:158:PRO:O   | 58:BZ:160:GLY:N   | 2.47                     | 0.41              |
| 1:CA:17:U:H1'     | 1:CA:1080:A:N3    | 2.35                     | 0.41              |
| 1:CA:1321:C:C4    | 1:CA:1322:C:C4    | 3.09                     | 0.41              |
| 1:CA:32:A:C6      | 1:CA:33:A:C6      | 3.09                     | 0.41              |
| 1:CA:437:U:H2'    | 1:CA:438:G:O4'    | 2.21                     | 0.41              |
| 1:CA:923:A:OP1    | 5:CE:21:ALA:HB2   | 2.21                     | 0.41              |
| 1:CA:943:U:H2'    | 1:CA:944:G:C5'    | 2.49                     | 0.41              |
| 2:CB:178:ARG:HD3  | 2:CB:178:ARG:HA   | 1.80                     | 0.41              |
| 9:CI:93:ARG:C     | 9:CI:95:LYS:N     | 2.74                     | 0.41              |
| 12:CL:105:TYR:C   | 12:CL:107:ALA:H   | 2.25                     | 0.41              |
| 13:CM:64:TRP:N    | 13:CM:64:TRP:CD1  | 2.89                     | 0.41              |
| 16:CP:75:ARG:HA   | 16:CP:80:PHE:HD1  | 1.85                     | 0.41              |
| 22:CW:69:C:C4     | 22:CW:70:C:N4     | 2.89                     | 0.41              |
| 24:CY:114:VAL:O   | 24:CY:114:VAL:CG1 | 2.66                     | 0.41              |
| 24:CY:252:ASP:O   | 24:CY:254:LYS:HE3 | 2.21                     | 0.41              |
| 27:D2:67:LYS:O    | 27:D2:69:ARG:N    | 2.53                     | 0.41              |
| 27:D2:4:SER:C     | 27:D2:6:VAL:N     | 2.74                     | 0.41              |
| 29:D4:16:CYS:HB3  | 29:D4:20:ASN:O    | 2.21                     | 0.41              |
| 29:D4:53:GLU:HB3  | 29:D4:55:ARG:CZ   | 2.50                     | 0.41              |
| 30:D5:2:ALA:O     | 30:D5:3:LYS:CB    | 2.69                     | 0.41              |
| 34:D9:29:ASN:OD1  | 34:D9:32:HIS:NE2  | 2.54                     | 0.41              |
| 35:DA:83:G:H22    | 35:DA:102:G:H2'   | 1.83                     | 0.41              |
| 35:DA:1174:A:H5'  | 35:DA:1175:U:H5'' | 2.02                     | 0.41              |
| 35:DA:1198:U:O2   | 35:DA:1198:U:C2'  | 2.69                     | 0.41              |
| 35:DA:1301:A:HO2' | 35:DA:1302:A:C2'  | 2.31                     | 0.41              |
| 35:DA:1491:G:N3   | 35:DA:1492:G:C8   | 2.89                     | 0.41              |
| 35:DA:1523:U:H2'  | 35:DA:1524:G:H8   | 1.81                     | 0.41              |
| 35:DA:1882:C:H2'  | 35:DA:1883:G:O4'  | 2.21                     | 0.41              |
| 31:D6:8:LYS:NZ    | 35:DA:2285:C:C5   | 2.76                     | 0.41              |
| 35:DA:234:C:H2'   | 35:DA:235:U:H6    | 1.86                     | 0.41              |
| 35:DA:2422:A:H3'  | 35:DA:2422:A:H8   | 1.86                     | 0.41              |
| 35:DA:676:A:C1'   | 35:DA:2443:C:H1'  | 2.45                     | 0.41              |
| 35:DA:2696:U:H2'  | 35:DA:2697:G:H8   | 1.86                     | 0.41              |
| 35:DA:2881:C:H2'  | 35:DA:2882:A:H8   | 1.87                     | 0.41              |
| 35:DA:2889:C:H2'  | 35:DA:2891:G:C8   | 2.56                     | 0.41              |
| 35:DA:327:G:N2    | 35:DA:328:U:H1'   | 2.36                     | 0.41              |
| 35:DA:481:G:N2    | 35:DA:507:A:H1'   | 2.35                     | 0.41              |
| 35:DA:557:U:H2'   | 35:DA:558:G:C8    | 2.55                     | 0.41              |
| 35:DA:570:G:O6    | 35:DA:2499:C:OP1  | 2.39                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:DA:910:A:C6    | 35:DA:911:A:C6     | 3.09                     | 0.41              |
| 36:DB:36:C:H2'    | 36:DB:37:C:C6      | 2.55                     | 0.41              |
| 38:DD:92:ILE:H    | 38:DD:92:ILE:CD1   | 2.34                     | 0.41              |
| 35:DA:2773:C:H5'' | 39:DE:164:ARG:HG2  | 2.03                     | 0.41              |
| 39:DE:107:THR:C   | 39:DE:190:GLY:HA2  | 2.36                     | 0.41              |
| 41:DG:140:ILE:H   | 41:DG:140:ILE:HG13 | 1.71                     | 0.41              |
| 41:DG:168:GLU:C   | 41:DG:170:ARG:N    | 2.74                     | 0.41              |
| 41:DG:34:LEU:CD1  | 41:DG:34:LEU:N     | 2.76                     | 0.41              |
| 41:DG:61:ALA:O    | 41:DG:64:THR:HG22  | 2.21                     | 0.41              |
| 41:DG:76:SER:CB   | 41:DG:83:ARG:HA    | 2.50                     | 0.41              |
| 41:DG:9:ARG:O     | 41:DG:10:LYS:C     | 2.60                     | 0.41              |
| 42:DH:136:ILE:O   | 42:DH:136:ILE:HG22 | 2.21                     | 0.41              |
| 42:DH:45:VAL:O    | 42:DH:47:GLU:N     | 2.54                     | 0.41              |
| 42:DH:66:GLY:O    | 42:DH:67:LEU:C     | 2.58                     | 0.41              |
| 45:DL:3:UNK:O     | 45:DL:7:UNK:CB     | 4.15                     | 0.41              |
| 35:DA:558:G:OP1   | 46:DN:111:PRO:HD2  | 2.20                     | 0.41              |
| 46:DN:57:ALA:HB3  | 46:DN:124:ALA:HA   | 2.01                     | 0.41              |
| 47:DO:91:LEU:N    | 47:DO:91:LEU:CD2   | 2.83                     | 0.41              |
| 49:DQ:68:ILE:CG2  | 49:DQ:103:MET:HA   | 2.51                     | 0.41              |
| 51:DS:35:ILE:HG22 | 51:DS:53:SER:HB2   | 2.02                     | 0.41              |
| 51:DS:42:ASP:O    | 51:DS:43:GLU:CB    | 2.69                     | 0.41              |
| 51:DS:24:LEU:CB   | 51:DS:85:VAL:HG12  | 2.38                     | 0.41              |
| 51:DS:92:TYR:CG   | 51:DS:93:LYS:N     | 2.89                     | 0.41              |
| 53:DU:10:ARG:C    | 53:DU:12:ARG:N     | 2.74                     | 0.41              |
| 53:DU:51:LYS:HA   | 53:DU:54:LYS:HE2   | 2.02                     | 0.41              |
| 56:DX:23:GLU:O    | 56:DX:25:LYS:N     | 2.48                     | 0.41              |
| 56:DX:35:THR:CG2  | 56:DX:36:LYS:N     | 2.83                     | 0.41              |
| 1:AA:1098:C:O2'   | 1:AA:1099:G:H5'    | 2.21                     | 0.40              |
| 1:AA:1493:A:O2'   | 1:AA:1494:G:OP1    | 2.33                     | 0.40              |
| 1:AA:1511:G:C2'   | 1:AA:1512:U:H5'    | 2.51                     | 0.40              |
| 1:AA:224:C:H2'    | 1:AA:225:C:C6      | 2.55                     | 0.40              |
| 1:AA:32:A:H3'     | 1:AA:33:A:H8       | 1.86                     | 0.40              |
| 1:AA:596:C:OP2    | 1:AA:597:G:OP2     | 2.39                     | 0.40              |
| 2:AB:110:GLN:H    | 2:AB:110:GLN:HG3   | 1.57                     | 0.40              |
| 3:AC:14:ILE:CG1   | 3:AC:15:THR:N      | 2.83                     | 0.40              |
| 3:AC:87:LEU:C     | 3:AC:89:GLU:N      | 2.69                     | 0.40              |
| 4:AD:121:VAL:N    | 4:AD:126:ILE:HD13  | 2.36                     | 0.40              |
| 4:AD:192:GLU:O    | 4:AD:194:LEU:N     | 2.54                     | 0.40              |
| 7:AG:52:GLU:O     | 7:AG:53:LYS:C      | 2.58                     | 0.40              |
| 8:AH:10:LEU:HD22  | 8:AH:83:ILE:CD1    | 2.45                     | 0.40              |
| 8:AH:56:LYS:HA    | 8:AH:57:PRO:HD2    | 1.82                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:AI:11:LYS:O      | 9:AI:12:GLU:HB2    | 2.21                     | 0.40              |
| 10:AJ:12:ASP:OD1   | 10:AJ:15:THR:HG23  | 2.21                     | 0.40              |
| 10:AJ:32:ALA:HB1   | 10:AJ:75:ILE:CG1   | 2.49                     | 0.40              |
| 10:AJ:4:ILE:HD11   | 10:AJ:77:PRO:HB3   | 2.03                     | 0.40              |
| 11:AK:93:GLN:O     | 11:AK:94:ALA:C     | 2.60                     | 0.40              |
| 12:AL:70:ILE:HG23  | 12:AL:100:ILE:HD12 | 2.03                     | 0.40              |
| 13:AM:119:GLY:C    | 13:AM:121:LYS:H    | 2.24                     | 0.40              |
| 13:AM:66:LEU:HA    | 13:AM:70:LEU:CD1   | 2.50                     | 0.40              |
| 16:AP:75:ARG:HG3   | 16:AP:75:ARG:HH11  | 1.86                     | 0.40              |
| 20:AT:63:ILE:C     | 20:AT:65:LYS:N     | 2.74                     | 0.40              |
| 22:AW:19:G:C6      | 22:AW:58:A:C6      | 3.08                     | 0.40              |
| 24:AY:104:ALA:O    | 24:AY:132:ARG:HB2  | 2.21                     | 0.40              |
| 24:AY:145:ASP:OD2  | 24:AY:148:LEU:HB2  | 2.21                     | 0.40              |
| 24:AY:168:ILE:HG23 | 24:AY:205:TYR:CE2  | 2.55                     | 0.40              |
| 24:AY:211:GLU:O    | 24:AY:215:LYS:HG3  | 2.20                     | 0.40              |
| 24:AY:300:GLU:O    | 24:AY:301:ILE:HD13 | 2.20                     | 0.40              |
| 24:AY:335:LEU:HD23 | 24:AY:355:LEU:HD11 | 2.03                     | 0.40              |
| 24:AY:468:ARG:C    | 24:AY:470:PHE:N    | 2.73                     | 0.40              |
| 24:AY:505:GLY:HA3  | 24:AY:576:ASP:OD1  | 2.20                     | 0.40              |
| 24:AY:679:VAL:O    | 24:AY:681:LYS:N    | 2.46                     | 0.40              |
| 26:B1:53:VAL:CG1   | 26:B1:54:ALA:N     | 2.83                     | 0.40              |
| 33:B8:50:LEU:HA    | 33:B8:53:PRO:HG3   | 2.04                     | 0.40              |
| 34:B9:29:ASN:HA    | 34:B9:30:PRO:HD2   | 1.89                     | 0.40              |
| 35:BA:1270:C:H5''  | 35:BA:1271:G:C5'   | 2.51                     | 0.40              |
| 35:BA:1668:A:H4'   | 35:BA:1669:A:O5'   | 2.20                     | 0.40              |
| 35:BA:1863:G:H2'   | 35:BA:1864:U:O4'   | 2.22                     | 0.40              |
| 35:BA:2242:G:N2    | 35:BA:2434:A:H2    | 2.19                     | 0.40              |
| 35:BA:2441:C:O2'   | 35:BA:2442:C:H5'   | 2.21                     | 0.40              |
| 35:BA:2657:A:O2'   | 42:BH:160:LYS:CE   | 2.68                     | 0.40              |
| 35:BA:2712:U:O2'   | 35:BA:2712(A):A:C8 | 2.42                     | 0.40              |
| 35:BA:2861:G:C4    | 35:BA:2862:G:C8    | 3.09                     | 0.40              |
| 32:B7:11:LYS:HE2   | 35:BA:686:G:H5''   | 2.03                     | 0.40              |
| 35:BA:71:A:H5''    | 35:BA:72:U:O5'     | 2.21                     | 0.40              |
| 35:BA:94:C:O2      | 35:BA:94:C:H2'     | 2.20                     | 0.40              |
| 35:BA:979:G:H2'    | 35:BA:982:C:H41    | 1.86                     | 0.40              |
| 37:BC:181:PHE:HA   | 37:BC:182:PRO:HD3  | 1.85                     | 0.40              |
| 37:BC:75:VAL:HG12  | 37:BC:76:LEU:N     | 2.36                     | 0.40              |
| 38:BD:266:SER:C    | 38:BD:267:SER:O    | 2.58                     | 0.40              |
| 39:BE:103:ASP:OD2  | 39:BE:168:MET:HE2  | 2.20                     | 0.40              |
| 39:BE:167:VAL:HG13 | 39:BE:170:LEU:HD11 | 2.03                     | 0.40              |
| 39:BE:29:GLY:O     | 39:BE:30:PRO:C     | 2.58                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:BE:38:THR:HG23  | 39:BE:39:PRO:HD2   | 2.02                     | 0.40              |
| 40:BF:132:VAL:O    | 40:BF:138:GLU:OE1  | 2.39                     | 0.40              |
| 41:BG:117:PHE:HE1  | 41:BG:119:GLY:C    | 2.24                     | 0.40              |
| 41:BG:125:PHE:CZ   | 41:BG:173:LEU:HD12 | 2.56                     | 0.40              |
| 42:BH:163:TYR:CD1  | 42:BH:163:TYR:N    | 2.89                     | 0.40              |
| 42:BH:89:ILE:HD13  | 42:BH:94:TYR:HB3   | 2.03                     | 0.40              |
| 46:BN:128:HIS:O    | 46:BN:130:HIS:N    | 2.54                     | 0.40              |
| 46:BN:3:THR:CG2    | 46:BN:4:TYR:H      | 2.27                     | 0.40              |
| 48:BP:121:LYS:HB2  | 48:BP:123:LEU:HD21 | 2.03                     | 0.40              |
| 48:BP:12:ALA:CB    | 48:BP:16:ARG:HB3   | 2.50                     | 0.40              |
| 49:BQ:70:PRO:CA    | 49:BQ:95:ALA:HB2   | 2.51                     | 0.40              |
| 50:BR:79:LEU:HD22  | 50:BR:83:ILE:HB    | 2.01                     | 0.40              |
| 35:BA:2334:G:N3    | 51:BS:18:ILE:HD13  | 2.36                     | 0.40              |
| 53:BU:78:THR:O     | 53:BU:79:PHE:C     | 2.59                     | 0.40              |
| 53:BU:95:LEU:HD13  | 54:BV:4:ILE:CG2    | 2.48                     | 0.40              |
| 58:BZ:56:VAL:HG13  | 58:BZ:69:THR:O     | 2.21                     | 0.40              |
| 1:CA:1121:U:O2'    | 1:CA:1122:U:H5'    | 2.22                     | 0.40              |
| 1:CA:1370:G:C2     | 1:CA:1371:G:N7     | 2.89                     | 0.40              |
| 1:CA:160:A:H1'     | 1:CA:344:A:C4      | 2.57                     | 0.40              |
| 1:CA:439:A:H2'     | 1:CA:441:A:C5'     | 2.51                     | 0.40              |
| 1:CA:476:G:H2'     | 1:CA:477:A:C8      | 2.56                     | 0.40              |
| 1:CA:707:C:H2'     | 1:CA:708:C:C6      | 2.55                     | 0.40              |
| 1:CA:740:U:O2'     | 1:CA:741:G:C5'     | 2.68                     | 0.40              |
| 1:CA:933:G:OP2     | 7:CG:3:ARG:HB3     | 2.21                     | 0.40              |
| 2:CB:130:ARG:HA    | 2:CB:131:PRO:HD2   | 1.84                     | 0.40              |
| 4:CD:53:ASP:O      | 4:CD:57:ARG:HD2    | 2.21                     | 0.40              |
| 10:CJ:24:VAL:C     | 10:CJ:26:ALA:N     | 2.75                     | 0.40              |
| 12:CL:28:LYS:HE2   | 12:CL:33:ARG:CZ    | 2.51                     | 0.40              |
| 1:CA:523:A:N1      | 12:CL:92:ASP:HB2   | 2.36                     | 0.40              |
| 12:CL:46:LYS:NZ    | 12:CL:94:PRO:HG3   | 2.35                     | 0.40              |
| 1:CA:1359:C:OP2    | 14:CN:22:THR:HG21  | 2.21                     | 0.40              |
| 17:CQ:45:HIS:HB2   | 17:CQ:65:ILE:CD1   | 2.51                     | 0.40              |
| 17:CQ:53:LEU:HD23  | 17:CQ:54:GLY:N     | 2.35                     | 0.40              |
| 24:CY:168:ILE:HD12 | 24:CY:176:GLY:CA   | 2.45                     | 0.40              |
| 24:CY:196:ILE:C    | 24:CY:196:ILE:HD12 | 2.41                     | 0.40              |
| 24:CY:219:VAL:HA   | 24:CY:222:ASP:OD2  | 2.22                     | 0.40              |
| 24:CY:227:ILE:HD13 | 24:CY:242:LEU:HD23 | 2.03                     | 0.40              |
| 24:CY:369:LEU:N    | 24:CY:369:LEU:CD1  | 2.84                     | 0.40              |
| 24:CY:530:VAL:CG1  | 24:CY:533:VAL:CG2  | 2.99                     | 0.40              |
| 24:CY:689:LYS:CG   | 24:CY:690:GLY:N    | 2.84                     | 0.40              |
| 24:CY:86:GLY:O     | 24:CY:88:VAL:N     | 2.54                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:CY:87:HIS:O     | 24:CY:88:VAL:C     | 2.59                     | 0.40              |
| 27:D2:59:ARG:HA    | 35:DA:76:C:HO2'    | 1.86                     | 0.40              |
| 35:DA:1042:G:C6    | 35:DA:1114:G:N1    | 2.89                     | 0.40              |
| 35:DA:1061:U:H4'   | 35:DA:1070:A:C1'   | 2.45                     | 0.40              |
| 35:DA:1061:U:H5''  | 35:DA:1062:G:OP2   | 2.20                     | 0.40              |
| 35:DA:1328:G:H2'   | 35:DA:1330:C:C5    | 2.56                     | 0.40              |
| 35:DA:1590:U:H2'   | 35:DA:1591:G:C8    | 2.56                     | 0.40              |
| 35:DA:13:A:H1'     | 35:DA:15:G:N7      | 2.36                     | 0.40              |
| 35:DA:1640:C:H2'   | 35:DA:1641:A:O4'   | 2.21                     | 0.40              |
| 35:DA:1788:C:H2'   | 35:DA:1789:A:C8    | 2.55                     | 0.40              |
| 35:DA:1973:G:H2'   | 35:DA:1974:C:C6    | 2.56                     | 0.40              |
| 35:DA:1999:C:H4'   | 35:DA:2723:C:O2    | 2.20                     | 0.40              |
| 35:DA:2488:A:H2'   | 35:DA:2489:G:C8    | 2.57                     | 0.40              |
| 35:DA:1669:A:O3'   | 35:DA:2549:G:H5'   | 2.22                     | 0.40              |
| 35:DA:2652:C:C4    | 35:DA:2653:U:C4    | 3.09                     | 0.40              |
| 35:DA:483:A:H3'    | 35:DA:484:C:H6     | 1.86                     | 0.40              |
| 35:DA:545:C:C3'    | 35:DA:547:A:C5'    | 2.95                     | 0.40              |
| 35:DA:646:A:H2'    | 35:DA:647:G:O4'    | 2.21                     | 0.40              |
| 35:DA:654(S):G:H3' | 35:DA:654(T):C:C4' | 2.51                     | 0.40              |
| 35:DA:695:G:N2     | 35:DA:696:G:H1'    | 2.36                     | 0.40              |
| 37:DC:132:LEU:O    | 37:DC:138:LEU:N    | 2.48                     | 0.40              |
| 39:DE:168:MET:CE   | 39:DE:202:LYS:HE2  | 2.51                     | 0.40              |
| 41:DG:105:LYS:H    | 41:DG:105:LYS:HG3  | 1.49                     | 0.40              |
| 41:DG:11:TYR:OH    | 41:DG:33:ARG:CB    | 2.69                     | 0.40              |
| 43:DJ:37:UNK:O     | 43:DJ:39:UNK:N     | 2.54                     | 0.40              |
| 43:DJ:58:UNK:O     | 43:DJ:61:UNK:N     | 2.53                     | 0.40              |
| 44:DK:27:LEU:HA    | 44:DK:30:HIS:HB2   | 2.02                     | 0.40              |
| 44:DK:93:ARG:HD2   | 44:DK:93:ARG:O     | 2.20                     | 0.40              |
| 46:DN:13:TRP:O     | 46:DN:135:PRO:HD2  | 2.21                     | 0.40              |
| 46:DN:35:ARG:HB3   | 46:DN:42:TRP:CZ3   | 2.56                     | 0.40              |
| 47:DO:64:ARG:NH1   | 47:DO:83:ALA:CB    | 2.83                     | 0.40              |
| 48:DP:50:ARG:HG3   | 48:DP:51:PHE:N     | 2.35                     | 0.40              |
| 48:DP:81:GLN:HE21  | 48:DP:81:GLN:HB2   | 1.67                     | 0.40              |
| 50:DR:28:LEU:HA    | 50:DR:34:ILE:CG1   | 2.51                     | 0.40              |
| 50:DR:3:HIS:O      | 50:DR:4:LEU:CB     | 2.69                     | 0.40              |
| 52:DT:55:ASN:HD22  | 52:DT:58:ASN:HD21  | 1.66                     | 0.40              |
| 47:DO:119:PRO:HB2  | 52:DT:68:TYR:CE2   | 2.56                     | 0.40              |
| 54:DV:35:LEU:HB2   | 54:DV:57:VAL:HG12  | 2.03                     | 0.40              |
| 55:DW:5:ALA:HB2    | 55:DW:54:ALA:CB    | 2.39                     | 0.40              |
| 55:DW:6:ILE:HA     | 55:DW:103:ILE:O    | 2.21                     | 0.40              |
| 56:DX:29:TRP:CZ3   | 56:DX:76:ARG:HB2   | 2.55                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:DZ:110:GLY:HA2  | 58:DZ:145:GLU:OE1  | 2.21                     | 0.40              |
| 1:AA:1351:U:O2'    | 1:AA:1352:C:H5'    | 2.22                     | 0.40              |
| 1:AA:313:A:H2'     | 1:AA:314:C:C6      | 2.56                     | 0.40              |
| 1:AA:427:U:C4      | 1:AA:428:G:C6      | 3.09                     | 0.40              |
| 1:AA:50:A:N6       | 1:AA:361:G:C4'     | 2.79                     | 0.40              |
| 1:AA:532:A:O2'     | 1:AA:533:A:P       | 2.78                     | 0.40              |
| 1:AA:538:G:H2'     | 1:AA:539:A:C8      | 2.56                     | 0.40              |
| 1:AA:556:C:O2'     | 1:AA:557:G:H5'     | 2.21                     | 0.40              |
| 1:AA:597:G:H1'     | 1:AA:644:G:N2      | 2.37                     | 0.40              |
| 1:AA:902:G:H2'     | 1:AA:903:G:H8      | 1.86                     | 0.40              |
| 1:AA:955:U:H2'     | 1:AA:956:U:C6      | 2.56                     | 0.40              |
| 2:AB:55:PHE:HD1    | 2:AB:221:LEU:HG    | 1.86                     | 0.40              |
| 3:AC:124:ILE:O     | 3:AC:124:ILE:HG22  | 2.21                     | 0.40              |
| 4:AD:36:ARG:CG     | 4:AD:36:ARG:NH1    | 2.83                     | 0.40              |
| 4:AD:53:ASP:O      | 4:AD:57:ARG:HD2    | 2.22                     | 0.40              |
| 4:AD:58:LEU:HD23   | 4:AD:62:GLN:HG2    | 2.03                     | 0.40              |
| 4:AD:62:GLN:O      | 4:AD:66:ARG:HD2    | 2.21                     | 0.40              |
| 5:AE:79:GLU:HB3    | 5:AE:93:PRO:CD     | 2.52                     | 0.40              |
| 6:AF:12:PRO:C      | 6:AF:14:LEU:H      | 2.22                     | 0.40              |
| 7:AG:80:VAL:CG2    | 7:AG:81:GLY:N      | 2.80                     | 0.40              |
| 8:AH:1:MET:O       | 8:AH:2:LEU:C       | 2.59                     | 0.40              |
| 10:AJ:50:ILE:HD11  | 14:AN:41:ARG:CZ    | 2.51                     | 0.40              |
| 11:AK:34:ASP:HB3   | 11:AK:40:ILE:HD11  | 2.03                     | 0.40              |
| 13:AM:16:ASP:HB3   | 13:AM:41:PRO:HB3   | 2.03                     | 0.40              |
| 16:AP:9:PHE:HE2    | 16:AP:18:ARG:NE    | 2.19                     | 0.40              |
| 17:AQ:10:VAL:HG13  | 17:AQ:19:VAL:HB    | 2.03                     | 0.40              |
| 1:AA:1320:C:N4     | 19:AS:36:ARG:HG3   | 2.36                     | 0.40              |
| 19:AS:45:VAL:O     | 19:AS:47:HIS:N     | 2.51                     | 0.40              |
| 20:AT:44:ALA:HA    | 20:AT:92:LEU:HD21  | 2.02                     | 0.40              |
| 24:AY:20:HIS:CE1   | 24:AY:21:ILE:HG12  | 2.57                     | 0.40              |
| 24:AY:216:LEU:CD2  | 24:AY:216:LEU:C    | 2.89                     | 0.40              |
| 24:AY:238:THR:HG22 | 24:AY:241:GLU:H    | 1.83                     | 0.40              |
| 24:AY:286:ILE:HG23 | 24:AY:287:PRO:HD2  | 2.04                     | 0.40              |
| 24:AY:304:ASP:C    | 24:AY:306:ASN:H    | 2.24                     | 0.40              |
| 24:AY:420:ASP:HB3  | 24:AY:472:VAL:HG13 | 2.02                     | 0.40              |
| 24:AY:486:THR:CG2  | 24:AY:600:VAL:HG13 | 2.50                     | 0.40              |
| 25:B0:20:ARG:NH1   | 25:B0:20:ARG:CG    | 2.84                     | 0.40              |
| 26:B1:53:VAL:HG12  | 26:B1:54:ALA:N     | 2.36                     | 0.40              |
| 27:B2:57:ILE:HG22  | 27:B2:61:LEU:CD1   | 2.51                     | 0.40              |
| 28:B3:4:LEU:HD23   | 28:B3:58:VAL:HA    | 2.02                     | 0.40              |
| 31:B6:12:GLU:HG2   | 31:B6:23:THR:CG2   | 2.52                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:BA:1061:U:H4'  | 35:BA:1070:A:C1'  | 2.45                     | 0.40              |
| 35:BA:1062:G:H22  | 35:BA:1077:A:H1'  | 1.86                     | 0.40              |
| 35:BA:1342:A:O2'  | 35:BA:1344:G:OP2  | 2.32                     | 0.40              |
| 35:BA:1345:C:C2'  | 35:BA:1346:G:H5'  | 2.50                     | 0.40              |
| 35:BA:1499:C:H2'  | 35:BA:1500:G:O4'  | 2.21                     | 0.40              |
| 35:BA:1523:U:H2'  | 35:BA:1524:G:H8   | 1.84                     | 0.40              |
| 35:BA:1664:A:OP1  | 35:BA:1665:A:OP2  | 2.39                     | 0.40              |
| 35:BA:2577:A:C5'  | 35:BA:2578:G:C5'  | 2.99                     | 0.40              |
| 35:BA:594:U:H2'   | 35:BA:595:C:C6    | 2.56                     | 0.40              |
| 35:BA:2122:U:O2'  | 37:BC:173:HIS:HD2 | 2.04                     | 0.40              |
| 37:BC:84:ILE:HG23 | 37:BC:95:VAL:HG12 | 2.02                     | 0.40              |
| 40:BF:68:LYS:HG3  | 40:BF:69:HIS:CD2  | 2.55                     | 0.40              |
| 42:BH:87:LEU:HD22 | 42:BH:163:TYR:O   | 2.21                     | 0.40              |
| 44:BK:52:ILE:HG22 | 44:BK:53:VAL:N    | 2.37                     | 0.40              |
| 48:BP:100:LEU:CD2 | 48:BP:100:LEU:N   | 2.84                     | 0.40              |
| 48:BP:81:GLN:HG2  | 48:BP:106:LEU:HA  | 2.02                     | 0.40              |
| 48:BP:107:LYS:HB2 | 48:BP:107:LYS:HE3 | 1.79                     | 0.40              |
| 48:BP:56:SER:O    | 48:BP:58:THR:N    | 2.54                     | 0.40              |
| 51:BS:65:VAL:C    | 51:BS:67:ARG:N    | 2.75                     | 0.40              |
| 53:BU:57:PHE:O    | 53:BU:59:ARG:N    | 2.54                     | 0.40              |
| 57:BY:18:GLY:O    | 57:BY:21:LYS:HB2  | 2.21                     | 0.40              |
| 57:BY:90:LEU:HB2  | 57:BY:91:GLU:OE2  | 2.20                     | 0.40              |
| 58:BZ:109:ALA:HB3 | 58:BZ:144:LEU:O   | 2.21                     | 0.40              |
| 58:BZ:99:TYR:CE2  | 58:BZ:125:LEU:HB2 | 2.56                     | 0.40              |
| 1:CA:1054:C:OP1   | 1:CA:1198:G:OP2   | 2.39                     | 0.40              |
| 1:CA:1329:A:C2'   | 1:CA:1330:U:H5'   | 2.51                     | 0.40              |
| 1:CA:1339:A:H2'   | 1:CA:1340:A:O4'   | 2.21                     | 0.40              |
| 1:CA:1397:C:H6    | 1:CA:1397:C:H3'   | 1.87                     | 0.40              |
| 1:CA:203:U:C4'    | 1:CA:204:U:OP1    | 2.70                     | 0.40              |
| 1:CA:244:U:C6     | 1:CA:894:G:C2     | 3.09                     | 0.40              |
| 1:CA:793:U:C3'    | 1:CA:794:A:C5'    | 2.90                     | 0.40              |
| 2:CB:32:ILE:O     | 2:CB:32:ILE:HG23  | 2.20                     | 0.40              |
| 2:CB:39:ILE:HG22  | 2:CB:41:ILE:HD12  | 2.02                     | 0.40              |
| 4:CD:65:ARG:HD3   | 4:CD:75:PHE:CD2   | 2.55                     | 0.40              |
| 7:CG:38:LEU:HD12  | 7:CG:38:LEU:O     | 2.22                     | 0.40              |
| 8:CH:114:THR:C    | 8:CH:116:LYS:N    | 2.74                     | 0.40              |
| 9:CI:56:LEU:HD23  | 9:CI:56:LEU:O     | 2.21                     | 0.40              |
| 9:CI:97:LYS:O     | 9:CI:98:PRO:C     | 2.58                     | 0.40              |
| 14:CN:23:ARG:CD   | 14:CN:28:GLY:O    | 2.65                     | 0.40              |
| 15:CO:82:ILE:O    | 15:CO:82:ILE:HD13 | 2.22                     | 0.40              |
| 19:CS:53:ASN:C    | 19:CS:55:LYS:N    | 2.75                     | 0.40              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:CS:58:VAL:O     | 19:CS:60:VAL:HG12  | 2.21                     | 0.40              |
| 20:CT:38:LYS:O     | 20:CT:39:LYS:C     | 2.59                     | 0.40              |
| 24:CY:128:TYR:HE2  | 24:CY:130:VAL:HG23 | 1.83                     | 0.40              |
| 24:CY:637:ARG:HG3  | 24:CY:642:VAL:CG2  | 2.51                     | 0.40              |
| 28:D3:59:VAL:CG1   | 28:D3:60:GLU:N     | 2.81                     | 0.40              |
| 29:D4:14:ILE:HG23  | 29:D4:31:ILE:HG22  | 2.03                     | 0.40              |
| 29:D4:49:PHE:O     | 29:D4:50:VAL:O     | 2.40                     | 0.40              |
| 29:D4:6:HIS:HB3    | 29:D4:7:PRO:CD     | 2.51                     | 0.40              |
| 35:DA:1320:C:H2'   | 35:DA:1329:U:OP2   | 2.21                     | 0.40              |
| 35:DA:1529:G:C6    | 35:DA:1541:G:N1    | 2.89                     | 0.40              |
| 35:DA:1741:A:H2'   | 35:DA:1742:G:O4'   | 2.20                     | 0.40              |
| 35:DA:1856:G:H1    | 35:DA:1886:C:H42   | 1.68                     | 0.40              |
| 35:DA:1907:G:C6    | 35:DA:1908:C:C4    | 3.09                     | 0.40              |
| 35:DA:2033:A:H2'   | 35:DA:2035:G:OP2   | 2.21                     | 0.40              |
| 35:DA:2202:C:H2'   | 38:DD:151:LYS:HZ3  | 1.86                     | 0.40              |
| 35:DA:2285:C:H5'   | 35:DA:2288:A:N6    | 2.36                     | 0.40              |
| 35:DA:271(P):C:H2' | 35:DA:271(Q):G:O4' | 2.20                     | 0.40              |
| 35:DA:511:U:C5     | 35:DA:512:G:C4     | 3.10                     | 0.40              |
| 35:DA:805:G:H5'    | 35:DA:806:C:C5     | 2.56                     | 0.40              |
| 36:DB:115:G:H2'    | 36:DB:116:G:C8     | 2.53                     | 0.40              |
| 36:DB:73:A:C8      | 36:DB:74:U:C5      | 3.09                     | 0.40              |
| 38:DD:136:ILE:HG22 | 38:DD:136:ILE:O    | 2.20                     | 0.40              |
| 38:DD:27:THR:CG2   | 38:DD:27:THR:O     | 2.70                     | 0.40              |
| 35:DA:2822:G:OP2   | 39:DE:110:GLY:O    | 2.39                     | 0.40              |
| 39:DE:165:VAL:HB   | 39:DE:189:PRO:CB   | 2.52                     | 0.40              |
| 39:DE:95:ILE:CD1   | 39:DE:95:ILE:H     | 2.32                     | 0.40              |
| 40:DF:182:ASN:ND2  | 40:DF:185:ASP:OD2  | 2.35                     | 0.40              |
| 40:DF:32:LEU:C     | 40:DF:32:LEU:CD2   | 2.87                     | 0.40              |
| 40:DF:61:GLY:O     | 40:DF:62:ARG:C     | 2.59                     | 0.40              |
| 41:DG:71:THR:HG23  | 41:DG:89:GLY:HA3   | 2.03                     | 0.40              |
| 44:DK:77:LEU:CD2   | 44:DK:77:LEU:N     | 2.77                     | 0.40              |
| 45:DL:112:UNK:O    | 45:DL:117:UNK:CB   | 2.69                     | 0.40              |
| 46:DN:91:LEU:O     | 46:DN:95:PRO:HB3   | 2.22                     | 0.40              |
| 48:DP:101:VAL:HG23 | 48:DP:102:ARG:N    | 2.36                     | 0.40              |
| 48:DP:38:GLN:CG    | 48:DP:39:LYS:H     | 2.04                     | 0.40              |
| 49:DQ:52:VAL:C     | 49:DQ:54:MET:N     | 2.74                     | 0.40              |
| 49:DQ:75:THR:CG2   | 49:DQ:76:LYS:H     | 2.34                     | 0.40              |
| 51:DS:97:ARG:CA    | 51:DS:97:ARG:HE    | 2.34                     | 0.40              |
| 52:DT:113:LYS:C    | 52:DT:114:LEU:HD23 | 2.42                     | 0.40              |
| 52:DT:57:PHE:C     | 52:DT:58:ASN:ND2   | 2.73                     | 0.40              |
| 52:DT:89:VAL:CB    | 52:DT:91:ARG:HG3   | 2.50                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:DU:53:ARG:O    | 53:DU:54:LYS:C    | 2.59                     | 0.40              |
| 53:DU:75:ASN:ND2  | 53:DU:77:SER:OG   | 2.54                     | 0.40              |
| 55:DW:62:HIS:O    | 55:DW:63:ASP:O    | 2.39                     | 0.40              |
| 57:DY:97:ARG:O    | 57:DY:98:VAL:HB   | 2.21                     | 0.40              |
| 58:DZ:157:LEU:O   | 58:DZ:158:PRO:O   | 2.39                     | 0.40              |
| 58:DZ:42:VAL:CG1  | 58:DZ:43:GLU:N    | 2.83                     | 0.40              |
| 1:AA:1002:G:H3'   | 1:AA:1003:G:C8    | 2.56                     | 0.40              |
| 1:AA:1053:G:O6    | 1:AA:1199:U:H2'   | 2.21                     | 0.40              |
| 1:AA:1319:A:OP1   | 19:AS:10:PHE:CZ   | 2.73                     | 0.40              |
| 1:AA:186:C:H2'    | 1:AA:187:C:C6     | 2.56                     | 0.40              |
| 1:AA:363:A:H5'    | 12:AL:34:ARG:HB2  | 2.02                     | 0.40              |
| 1:AA:894:G:H2'    | 1:AA:895:G:O4'    | 2.22                     | 0.40              |
| 1:AA:946:A:H3'    | 1:AA:947:G:C8     | 2.56                     | 0.40              |
| 2:AB:152:PHE:O    | 2:AB:152:PHE:HD1  | 2.04                     | 0.40              |
| 2:AB:204:ASN:ND2  | 2:AB:207:ALA:H    | 2.19                     | 0.40              |
| 2:AB:21:ARG:HB3   | 2:AB:39:ILE:HG12  | 2.02                     | 0.40              |
| 2:AB:95:GLN:HA    | 2:AB:95:GLN:OE1   | 2.22                     | 0.40              |
| 3:AC:134:ILE:O    | 3:AC:136:GLN:N    | 2.54                     | 0.40              |
| 4:AD:28:SER:HB3   | 4:AD:29:PRO:CD    | 2.49                     | 0.40              |
| 4:AD:4:TYR:CG     | 4:AD:5:ILE:N      | 2.86                     | 0.40              |
| 4:AD:6:GLY:O      | 4:AD:7:PRO:C      | 2.60                     | 0.40              |
| 5:AE:124:GLY:O    | 5:AE:125:SER:C    | 2.59                     | 0.40              |
| 5:AE:78:HIS:HE1   | 5:AE:80:ILE:CG2   | 2.34                     | 0.40              |
| 8:AH:6:ILE:H      | 8:AH:6:ILE:HD12   | 1.81                     | 0.40              |
| 10:AJ:79:ARG:NH1  | 10:AJ:79:ARG:HG2  | 2.36                     | 0.40              |
| 13:AM:117:VAL:O   | 13:AM:118:ALA:O   | 2.38                     | 0.40              |
| 15:AO:9:GLN:C     | 15:AO:11:VAL:N    | 2.75                     | 0.40              |
| 16:AP:6:LEU:HA    | 16:AP:6:LEU:HD12  | 1.89                     | 0.40              |
| 1:AA:238:G:P      | 17:AQ:25:ARG:HH22 | 2.44                     | 0.40              |
| 7:AG:82:GLY:CA    | 23:AX:13:A:H2     | 2.32                     | 0.40              |
| 24:AY:487:ILE:HB  | 24:AY:597:GLY:O   | 2.21                     | 0.40              |
| 27:B2:31:GLU:O    | 27:B2:35:LEU:N    | 2.46                     | 0.40              |
| 28:B3:22:ALA:CA   | 28:B3:46:ASN:HD22 | 2.34                     | 0.40              |
| 29:B4:16:CYS:HB3  | 29:B4:20:ASN:O    | 2.21                     | 0.40              |
| 29:B4:6:HIS:HB3   | 29:B4:7:PRO:CD    | 2.51                     | 0.40              |
| 34:B9:10:ILE:HG13 | 34:B9:10:ILE:H    | 1.74                     | 0.40              |
| 35:BA:1053:C:H2'  | 35:BA:1054:A:O4'  | 2.22                     | 0.40              |
| 35:BA:1073:A:H2'  | 35:BA:1074:G:H5'  | 2.02                     | 0.40              |
| 35:BA:1131:G:OP1  | 46:BN:80:GLY:N    | 2.49                     | 0.40              |
| 35:BA:1175:U:P    | 35:BA:1176:G:H5'' | 2.61                     | 0.40              |
| 35:BA:1917:U:H2'  | 35:BA:1918:A:C5'  | 2.51                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BA:2026:C:C4    | 35:BA:2027:G:C8    | 3.09                     | 0.40              |
| 35:BA:205:G:HO2'   | 35:BA:206:U:P      | 2.42                     | 0.40              |
| 35:BA:216:A:C4     | 35:BA:432:A:C2     | 3.10                     | 0.40              |
| 22:AW:77:A:H61     | 35:BA:2422:A:H5''  | 1.86                     | 0.40              |
| 35:BA:272(J):C:N4  | 35:BA:363:G:H22    | 2.20                     | 0.40              |
| 35:BA:2741:A:H2'   | 35:BA:2742:C:O4'   | 2.22                     | 0.40              |
| 35:BA:2841:C:O2'   | 35:BA:2842:G:H5'   | 2.21                     | 0.40              |
| 35:BA:2850:A:H2    | 50:BR:61:HIS:CD2   | 2.39                     | 0.40              |
| 35:BA:321:G:N2     | 35:BA:341:G:H5''   | 2.36                     | 0.40              |
| 35:BA:341:G:H2'    | 35:BA:342:G:C8     | 2.56                     | 0.40              |
| 35:BA:461:C:N4     | 35:BA:469:G:N2     | 2.69                     | 0.40              |
| 35:BA:511:U:H5     | 35:BA:512:G:C5     | 2.39                     | 0.40              |
| 35:BA:523:C:H6     | 35:BA:523:C:H3'    | 1.87                     | 0.40              |
| 35:BA:260:G:C1'    | 35:BA:621:A:H1'    | 2.52                     | 0.40              |
| 35:BA:654(L):G:C2' | 35:BA:654(M):C:H4' | 2.51                     | 0.40              |
| 35:BA:654(O):G:H2' | 35:BA:654(P):C:C5  | 2.56                     | 0.40              |
| 35:BA:700:G:H2'    | 35:BA:701:G:H8     | 1.85                     | 0.40              |
| 35:BA:746:A:H2'    | 35:BA:2612:C:H5''  | 2.03                     | 0.40              |
| 35:BA:887:A:N3     | 35:BA:887:A:H2'    | 2.37                     | 0.40              |
| 37:BC:37:LYS:O     | 37:BC:38:PHE:HB3   | 2.21                     | 0.40              |
| 35:BA:729:G:C5     | 38:BD:208:LYS:HB2  | 2.56                     | 0.40              |
| 39:BE:28:ALA:CB    | 39:BE:93:VAL:HG22  | 2.51                     | 0.40              |
| 40:BF:63:LYS:HA    | 40:BF:76:GLY:O     | 2.21                     | 0.40              |
| 41:BG:14:GLU:C     | 41:BG:17:PRO:HD2   | 2.41                     | 0.40              |
| 41:BG:71:THR:HG23  | 41:BG:90:LEU:CA    | 2.51                     | 0.40              |
| 41:BG:7:LEU:O      | 41:BG:8:LYS:C      | 2.58                     | 0.40              |
| 42:BH:124:GLU:HB2  | 42:BH:132:ARG:CG   | 2.49                     | 0.40              |
| 42:BH:46:GLU:HG3   | 42:BH:51:ARG:CB    | 2.51                     | 0.40              |
| 44:BK:104:VAL:CG2  | 44:BK:127:ILE:HB   | 2.51                     | 0.40              |
| 48:BP:119:GLU:CA   | 48:BP:119:GLU:OE1  | 2.69                     | 0.40              |
| 48:BP:6:LEU:HG     | 48:BP:7:ARG:H      | 1.84                     | 0.40              |
| 49:BQ:68:ILE:CG2   | 49:BQ:103:MET:HA   | 2.52                     | 0.40              |
| 50:BR:30:THR:HA    | 50:BR:78:LYS:HZ3   | 1.85                     | 0.40              |
| 50:BR:85:PRO:C     | 50:BR:87:TYR:N     | 2.73                     | 0.40              |
| 51:BS:74:ALA:HB2   | 51:BS:101:LEU:HD21 | 2.03                     | 0.40              |
| 51:BS:66:ALA:O     | 51:BS:99:LYS:HD3   | 2.21                     | 0.40              |
| 52:BT:8:LYS:C      | 52:BT:10:VAL:H     | 2.23                     | 0.40              |
| 52:BT:55:ASN:ND2   | 52:BT:55:ASN:O     | 2.55                     | 0.40              |
| 55:BW:62:HIS:O     | 55:BW:63:ASP:O     | 2.39                     | 0.40              |
| 57:BY:30:VAL:HG12  | 57:BY:31:LEU:N     | 2.37                     | 0.40              |
| 57:BY:76:CYS:O     | 57:BY:77:PRO:C     | 2.60                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:BZ:175:VAL:HB   | 58:BZ:176:PRO:CD   | 2.52                     | 0.40              |
| 1:CA:1053:G:C4     | 1:CA:1199:U:C5     | 3.09                     | 0.40              |
| 1:CA:1424:C:O2'    | 1:CA:1425:U:H5'    | 2.21                     | 0.40              |
| 1:CA:1511:G:H8     | 1:CA:1511:G:O5'    | 2.03                     | 0.40              |
| 1:CA:321:A:C2      | 1:CA:333:G:C2      | 3.09                     | 0.40              |
| 1:CA:841:U:H3'     | 1:CA:848:C:O4'     | 2.21                     | 0.40              |
| 1:CA:908:A:O2'     | 1:CA:909:A:H5'     | 2.22                     | 0.40              |
| 2:CB:97:TRP:CH2    | 2:CB:176:GLU:OE2   | 2.74                     | 0.40              |
| 3:CC:134:ILE:O     | 3:CC:135:LYS:C     | 2.59                     | 0.40              |
| 3:CC:149:ALA:HA    | 3:CC:201:TYR:O     | 2.22                     | 0.40              |
| 5:CE:51:VAL:O      | 5:CE:52:PRO:C      | 2.58                     | 0.40              |
| 8:CH:107:LEU:HA    | 8:CH:107:LEU:HD23  | 1.88                     | 0.40              |
| 8:CH:26:VAL:HG23   | 8:CH:27:PRO:HD2    | 2.02                     | 0.40              |
| 9:CI:60:ASP:O      | 9:CI:61:ALA:C      | 2.60                     | 0.40              |
| 11:CK:99:GLN:HG2   | 11:CK:105:VAL:HG21 | 2.03                     | 0.40              |
| 15:CO:33:THR:HG23  | 15:CO:63:ARG:HH12  | 1.86                     | 0.40              |
| 17:CQ:53:LEU:HD23  | 17:CQ:53:LEU:C     | 2.42                     | 0.40              |
| 19:CS:4:SER:O      | 19:CS:5:LEU:C      | 2.60                     | 0.40              |
| 20:CT:64:ASP:OD1   | 20:CT:81:LYS:HD2   | 2.21                     | 0.40              |
| 20:CT:84:LEU:C     | 20:CT:86:ARG:N     | 2.72                     | 0.40              |
| 22:CV:4:G:O2'      | 22:CV:5:G:H8       | 2.03                     | 0.40              |
| 7:CG:82:GLY:CA     | 23:CX:13:A:H2      | 2.33                     | 0.40              |
| 24:CY:265:LYS:C    | 24:CY:267:LYS:H    | 2.25                     | 0.40              |
| 24:CY:309:LEU:O    | 24:CY:390:VAL:HA   | 2.21                     | 0.40              |
| 24:CY:448:GLN:HE22 | 24:CY:480:GLN:NE2  | 2.18                     | 0.40              |
| 24:CY:507:TYR:O    | 24:CY:577:SER:HA   | 2.21                     | 0.40              |
| 26:D1:30:VAL:CG2   | 26:D1:31:GLY:N     | 2.76                     | 0.40              |
| 31:D6:5:VAL:CG2    | 35:DA:2283:C:OP1   | 2.70                     | 0.40              |
| 35:DA:1051:G:C4    | 35:DA:1052:C:N4    | 2.89                     | 0.40              |
| 35:DA:1226:A:H2'   | 35:DA:1227:G:H5'   | 2.04                     | 0.40              |
| 35:DA:1270:C:H5''  | 35:DA:1271:G:C5'   | 2.51                     | 0.40              |
| 35:DA:1398:C:H2'   | 35:DA:1399:C:C6    | 2.55                     | 0.40              |
| 35:DA:1993:U:C5'   | 39:DE:128:SER:HB3  | 2.52                     | 0.40              |
| 35:DA:2354:G:H2'   | 35:DA:2355:C:H6    | 1.86                     | 0.40              |
| 35:DA:2076:U:C5    | 35:DA:2596:U:C2    | 3.08                     | 0.40              |
| 35:DA:665:C:O5'    | 35:DA:665:C:H6     | 2.05                     | 0.40              |
| 35:DA:827:U:H4'    | 35:DA:828:U:O2     | 2.21                     | 0.40              |
| 35:DA:854:G:H1     | 35:DA:923:C:H42    | 1.70                     | 0.40              |
| 35:DA:915:C:H2'    | 35:DA:916:G:C8     | 2.56                     | 0.40              |
| 35:DA:979:G:H2'    | 35:DA:982:C:H41    | 1.87                     | 0.40              |
| 37:DC:181:PHE:HA   | 37:DC:182:PRO:HD3  | 1.84                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:DC:3:LYS:O      | 37:DC:3:LYS:HD3    | 2.21                     | 0.40              |
| 37:DC:30:VAL:HG11  | 37:DC:42:VAL:HG13  | 2.04                     | 0.40              |
| 38:DD:165:ILE:HD13 | 38:DD:175:LEU:CD2  | 2.51                     | 0.40              |
| 39:DE:96:PHE:O     | 39:DE:175:VAL:HG11 | 2.21                     | 0.40              |
| 40:DF:118:ALA:HA   | 40:DF:123:LEU:HB3  | 2.03                     | 0.40              |
| 41:DG:47:LYS:HB3   | 41:DG:48:GLU:H     | 1.69                     | 0.40              |
| 41:DG:5:VAL:CB     | 41:DG:8:LYS:HB2    | 2.43                     | 0.40              |
| 42:DH:41:MET:HG3   | 42:DH:42:ARG:N     | 2.36                     | 0.40              |
| 44:DK:5:VAL:HA     | 44:DK:59:ILE:HG23  | 2.02                     | 0.40              |
| 47:DO:104:ARG:CZ   | 52:DT:33:LYS:HD2   | 2.50                     | 0.40              |
| 33:D8:25:MET:HB2   | 48:DP:62:LEU:HD21  | 2.04                     | 0.40              |
| 49:DQ:26:TYR:CD1   | 49:DQ:140:ALA:HB3  | 2.57                     | 0.40              |
| 52:DT:32:TYR:O     | 52:DT:33:LYS:HB2   | 2.22                     | 0.40              |
| 52:DT:30:VAL:HG22  | 52:DT:84:GLN:O     | 2.22                     | 0.40              |
| 54:DV:38:LEU:HD12  | 54:DV:56:SER:CA    | 2.51                     | 0.40              |
| 54:DV:39:LEU:HD13  | 54:DV:51:VAL:HA    | 2.01                     | 0.40              |
| 57:DY:52:SER:O     | 57:DY:53:PRO:C     | 2.60                     | 0.40              |
| 57:DY:87:LYS:HB3   | 57:DY:87:LYS:HE2   | 1.90                     | 0.40              |
| 57:DY:7:VAL:HG11   | 57:DY:8:LYS:HZ1    | 1.85                     | 0.40              |
| 58:DZ:10:ARG:HD2   | 58:DZ:36:LYS:HB3   | 2.04                     | 0.40              |
| 58:DZ:34:ASN:O     | 58:DZ:35:ARG:HG2   | 2.21                     | 0.40              |
| 1:AA:1094:G:HO2'   | 1:AA:1095:U:P      | 2.45                     | 0.40              |
| 1:AA:1157:A:C1'    | 1:AA:1181:G:H21    | 2.35                     | 0.40              |
| 1:AA:1481:U:H2'    | 1:AA:1482:G:C8     | 2.57                     | 0.40              |
| 1:AA:157:G:C2      | 1:AA:165:C:C2      | 3.08                     | 0.40              |
| 1:AA:532:A:C2'     | 1:AA:533:A:OP1     | 2.69                     | 0.40              |
| 1:AA:631:G:H5'     | 1:AA:631:G:C8      | 2.52                     | 0.40              |
| 1:AA:671:G:N2      | 1:AA:736:C:C2      | 2.89                     | 0.40              |
| 2:AB:165:VAL:CG2   | 2:AB:166:ASP:N     | 2.73                     | 0.40              |
| 3:AC:9:GLY:HA2     | 3:AC:12:LEU:HG     | 2.03                     | 0.40              |
| 4:AD:25:ARG:C      | 4:AD:27:TYR:N      | 2.75                     | 0.40              |
| 5:AE:149:GLU:O     | 5:AE:153:LYS:HE2   | 2.21                     | 0.40              |
| 7:AG:120:ILE:O     | 7:AG:124:LEU:HB2   | 2.21                     | 0.40              |
| 7:AG:46:ALA:O      | 7:AG:49:ILE:N      | 2.55                     | 0.40              |
| 8:AH:97:VAL:HG13   | 8:AH:98:LYS:N      | 2.35                     | 0.40              |
| 9:AI:114:TYR:HD2   | 9:AI:114:TYR:N     | 2.20                     | 0.40              |
| 10:AJ:24:VAL:C     | 10:AJ:26:ALA:N     | 2.73                     | 0.40              |
| 11:AK:41:THR:HG23  | 11:AK:41:THR:O     | 2.21                     | 0.40              |
| 12:AL:60:LEU:CD2   | 12:AL:60:LEU:N     | 2.83                     | 0.40              |
| 13:AM:64:TRP:CD1   | 13:AM:64:TRP:N     | 2.88                     | 0.40              |
| 14:AN:24:CYS:SG    | 14:AN:39:LEU:HA    | 2.61                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:AP:74:LEU:O     | 16:AP:77:ALA:HB3   | 2.22                     | 0.40              |
| 18:AR:36:ASN:O     | 18:AR:39:VAL:HG23  | 2.22                     | 0.40              |
| 22:AW:6:G:H2'      | 22:AW:7:G:O4'      | 2.21                     | 0.40              |
| 24:AY:496:LYS:HA   | 24:AY:509:HIS:HB2  | 2.04                     | 0.40              |
| 24:AY:590:ILE:O    | 24:AY:592:GLU:N    | 2.53                     | 0.40              |
| 61:AY:702:FUA:H72  | 61:AY:702:FUA:H212 | 1.88                     | 0.40              |
| 24:AY:78:ARG:HH11  | 24:AY:78:ARG:HG3   | 1.87                     | 0.40              |
| 27:B2:38:GLN:NE2   | 27:B2:44:LEU:HB2   | 2.36                     | 0.40              |
| 28:B3:12:PRO:O     | 28:B3:13:ILE:C     | 2.58                     | 0.40              |
| 28:B3:22:ALA:HA    | 28:B3:46:ASN:HD22  | 1.86                     | 0.40              |
| 31:B6:27:LYS:HB3   | 31:B6:30:THR:CG2   | 2.51                     | 0.40              |
| 31:B6:8:LYS:O      | 31:B6:9:LEU:O      | 2.39                     | 0.40              |
| 35:BA:1024:G:OP2   | 35:BA:1026:U:OP1   | 2.38                     | 0.40              |
| 35:BA:1156:A:O2'   | 35:BA:1157:G:P     | 2.80                     | 0.40              |
| 35:BA:13:A:H1'     | 35:BA:15:G:N7      | 2.37                     | 0.40              |
| 35:BA:1680:U:C2'   | 35:BA:1681:G:H5'   | 2.51                     | 0.40              |
| 35:BA:1819:A:O2'   | 35:BA:1820:U:OP2   | 2.33                     | 0.40              |
| 35:BA:2031:A:N3    | 35:BA:2455:G:O2'   | 2.53                     | 0.40              |
| 35:BA:2174:C:O2'   | 35:BA:2175:C:H5'   | 2.21                     | 0.40              |
| 35:BA:2193:G:O2'   | 35:BA:2194:G:H5'   | 2.22                     | 0.40              |
| 35:BA:2412:A:N6    | 35:BA:2413:G:C2    | 2.89                     | 0.40              |
| 35:BA:2422:A:H3'   | 35:BA:2422:A:C8    | 2.57                     | 0.40              |
| 35:BA:2582:G:H2'   | 35:BA:2582:G:N3    | 2.35                     | 0.40              |
| 35:BA:2653:U:O2'   | 42:BH:110:SER:CB   | 2.69                     | 0.40              |
| 35:BA:266:G:O6     | 35:BA:267:C:C4     | 2.75                     | 0.40              |
| 35:BA:307:G:N2     | 35:BA:310:A:O5'    | 2.55                     | 0.40              |
| 35:BA:311:A:O4'    | 35:BA:332:A:C4     | 2.74                     | 0.40              |
| 35:BA:332:A:C6     | 35:BA:335:C:C2     | 3.10                     | 0.40              |
| 35:BA:613:G:C2     | 35:BA:615:G:C5     | 3.09                     | 0.40              |
| 35:BA:752:A:H4'    | 35:BA:753:C:O5'    | 2.22                     | 0.40              |
| 37:BC:100:ILE:O    | 37:BC:102:GLN:N    | 2.54                     | 0.40              |
| 37:BC:149:ASN:HD22 | 37:BC:149:ASN:C    | 2.24                     | 0.40              |
| 37:BC:154:ILE:HA   | 37:BC:157:ILE:HD12 | 2.03                     | 0.40              |
| 37:BC:29:LEU:O     | 37:BC:32:GLU:N     | 2.43                     | 0.40              |
| 35:BA:1568:G:H4'   | 38:BD:59:LYS:HB3   | 2.04                     | 0.40              |
| 39:BE:16:ARG:O     | 39:BE:18:ASP:N     | 2.55                     | 0.40              |
| 39:BE:167:VAL:HG22 | 39:BE:170:LEU:HD11 | 2.02                     | 0.40              |
| 40:BF:10:PRO:CG    | 40:BF:13:SER:OG    | 2.69                     | 0.40              |
| 41:BG:139:LEU:HA   | 41:BG:144:ILE:HD13 | 2.04                     | 0.40              |
| 41:BG:119:GLY:CA   | 41:BG:181:ARG:H    | 2.35                     | 0.40              |
| 41:BG:41:GLN:NE2   | 41:BG:60:LEU:HD21  | 2.37                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 42:BH:83:TYR:CB   | 42:BH:135:GLY:H    | 2.27                     | 0.40              |
| 42:BH:66:GLY:O    | 42:BH:67:LEU:C     | 2.58                     | 0.40              |
| 44:BK:57:ILE:CD1  | 44:BK:57:ILE:H     | 2.30                     | 0.40              |
| 44:BK:61:ALA:O    | 44:BK:63:ARG:N     | 2.55                     | 0.40              |
| 46:BN:55:VAL:CG2  | 46:BN:127:ASP:N    | 2.83                     | 0.40              |
| 46:BN:94:HIS:HA   | 46:BN:96:GLU:OE1   | 2.21                     | 0.40              |
| 1:AA:1423:G:OP1   | 47:BO:49:ARG:NH2   | 2.55                     | 0.40              |
| 52:BT:19:LEU:HA   | 52:BT:20:PRO:HD3   | 1.80                     | 0.40              |
| 53:BU:17:ILE:C    | 53:BU:19:LYS:N     | 2.75                     | 0.40              |
| 53:BU:99:ALA:HB2  | 53:BU:106:PHE:CZ   | 2.56                     | 0.40              |
| 35:BA:1334:G:O3'  | 56:BX:65:ARG:NH2   | 2.55                     | 0.40              |
| 57:BY:87:LYS:O    | 57:BY:88:LYS:HB2   | 2.20                     | 0.40              |
| 58:BZ:67:LEU:HD23 | 58:BZ:90:VAL:CG1   | 2.51                     | 0.40              |
| 58:BZ:80:ARG:O    | 58:BZ:81:ARG:C     | 2.59                     | 0.40              |
| 1:CA:109:A:C6     | 1:CA:326:G:C6      | 3.08                     | 0.40              |
| 1:CA:1228:C:C5    | 1:CA:1229:A:N7     | 2.90                     | 0.40              |
| 1:CA:1342:C:H1'   | 9:CI:124:GLN:CG    | 2.52                     | 0.40              |
| 1:CA:315:A:O2'    | 1:CA:316:G:P       | 2.79                     | 0.40              |
| 1:CA:625:G:C4     | 1:CA:626:U:C5      | 3.09                     | 0.40              |
| 1:CA:725:G:O2'    | 1:CA:726:C:H5'     | 2.21                     | 0.40              |
| 1:CA:778:G:H1'    | 11:CK:119:CYS:HB3  | 2.03                     | 0.40              |
| 1:CA:975:A:H4'    | 1:CA:976:G:C5'     | 2.33                     | 0.40              |
| 2:CB:236:TYR:O    | 2:CB:237:ALA:C     | 2.60                     | 0.40              |
| 2:CB:58:ILE:O     | 2:CB:61:LEU:N      | 2.47                     | 0.40              |
| 4:CD:61:LYS:HG3   | 4:CD:203:VAL:HG13  | 2.02                     | 0.40              |
| 5:CE:105:VAL:O    | 5:CE:106:PRO:C     | 2.58                     | 0.40              |
| 5:CE:81:GLU:HA    | 5:CE:89:ILE:O      | 2.21                     | 0.40              |
| 7:CG:146:GLU:O    | 7:CG:147:ALA:C     | 2.60                     | 0.40              |
| 8:CH:35:ILE:HG22  | 8:CH:39:LEU:CD2    | 2.51                     | 0.40              |
| 11:CK:34:ASP:OD2  | 11:CK:34:ASP:C     | 2.59                     | 0.40              |
| 11:CK:34:ASP:HB2  | 11:CK:35:PRO:HD2   | 2.03                     | 0.40              |
| 12:CL:17:LYS:CD   | 12:CL:18:VAL:HG22  | 2.47                     | 0.40              |
| 13:CM:68:GLY:O    | 13:CM:70:LEU:N     | 2.52                     | 0.40              |
| 18:CR:63:GLN:OE1  | 18:CR:63:GLN:HA    | 2.21                     | 0.40              |
| 24:CY:122:TRP:O   | 24:CY:124:GLN:N    | 2.55                     | 0.40              |
| 24:CY:141:LYS:O   | 24:CY:144:ALA:CB   | 2.69                     | 0.40              |
| 24:CY:171:GLU:HG3 | 24:CY:172:ASP:N    | 2.37                     | 0.40              |
| 24:CY:35:TYR:HB2  | 24:CY:273:LEU:HD11 | 2.04                     | 0.40              |
| 25:D0:24:LYS:HA   | 25:D0:24:LYS:HD3   | 1.93                     | 0.40              |
| 26:D1:17:SER:HB3  | 26:D1:38:SER:OG    | 2.22                     | 0.40              |
| 26:D1:43:TYR:CD1  | 26:D1:43:TYR:N     | 2.89                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:D2:24:LEU:HD13  | 27:D2:60:LEU:HD21  | 2.02                     | 0.40              |
| 31:D6:11:LEU:HA    | 31:D6:54:ILE:O     | 2.22                     | 0.40              |
| 31:D6:8:LYS:HA     | 31:D6:27:LYS:HA    | 2.02                     | 0.40              |
| 33:D8:32:LEU:HB2   | 33:D8:36:LYS:HD2   | 2.03                     | 0.40              |
| 35:DA:1005:C:OP2   | 35:DA:1011:G:H2'   | 2.22                     | 0.40              |
| 35:DA:1053:C:H2'   | 35:DA:1054:A:O4'   | 2.21                     | 0.40              |
| 35:DA:1277:G:O2'   | 50:DR:24:GLN:HG2   | 2.20                     | 0.40              |
| 35:DA:1314:C:H6    | 35:DA:1314:C:C5'   | 2.26                     | 0.40              |
| 35:DA:1434:A:H2'   | 35:DA:1434:A:N3    | 2.36                     | 0.40              |
| 35:DA:1608:A:C6    | 35:DA:1611:C:C2    | 3.09                     | 0.40              |
| 35:DA:1789:A:H2'   | 35:DA:1790:C:O4'   | 2.21                     | 0.40              |
| 35:DA:204:A:OP1    | 35:DA:204:A:H8     | 2.04                     | 0.40              |
| 35:DA:206:U:O2     | 35:DA:206:U:C2'    | 2.69                     | 0.40              |
| 35:DA:2392:A:H2    | 35:DA:2424:C:N4    | 2.19                     | 0.40              |
| 35:DA:2474:C:H5'   | 35:DA:2475:C:C5    | 2.56                     | 0.40              |
| 35:DA:2693:A:C6    | 35:DA:2717:G:C6    | 3.09                     | 0.40              |
| 35:DA:272(J):C:H3' | 35:DA:274:G:C5'    | 2.32                     | 0.40              |
| 35:DA:2880:C:H6    | 35:DA:2880:C:O5'   | 2.05                     | 0.40              |
| 35:DA:332:A:O2'    | 35:DA:333:G:P      | 2.80                     | 0.40              |
| 35:DA:654(O):G:H2' | 35:DA:654(P):C:C5  | 2.56                     | 0.40              |
| 35:DA:883:G:N2     | 35:DA:894:C:C2     | 2.89                     | 0.40              |
| 35:DA:820:A:N3     | 35:DA:943:U:H4'    | 2.37                     | 0.40              |
| 37:DC:154:ILE:HA   | 37:DC:157:ILE:HD12 | 2.04                     | 0.40              |
| 37:DC:16:ASP:HA    | 37:DC:17:PRO:HD2   | 1.86                     | 0.40              |
| 38:DD:92:ILE:HA    | 38:DD:107:ALA:H    | 1.87                     | 0.40              |
| 38:DD:150:LYS:HA   | 38:DD:150:LYS:HD3  | 1.98                     | 0.40              |
| 38:DD:226:MET:HB3  | 38:DD:230:ASP:CB   | 2.48                     | 0.40              |
| 38:DD:35:LYS:HA    | 38:DD:64:ILE:H     | 1.86                     | 0.40              |
| 39:DE:144:ARG:HB3  | 39:DE:145:LYS:H    | 1.57                     | 0.40              |
| 39:DE:31:CYS:HA    | 39:DE:32:PRO:HD3   | 1.82                     | 0.40              |
| 39:DE:36:ARG:HH21  | 39:DE:88:GLY:N     | 2.20                     | 0.40              |
| 39:DE:55:ASN:C     | 39:DE:57:LYS:N     | 2.74                     | 0.40              |
| 40:DF:29:ASN:HB3   | 40:DF:32:LEU:HB3   | 2.03                     | 0.40              |
| 41:DG:46:ALA:HA    | 41:DG:51:ARG:CB    | 2.51                     | 0.40              |
| 43:DJ:123:UNK:O    | 43:DJ:124:UNK:C    | 2.69                     | 0.40              |
| 44:DK:61:ALA:C     | 44:DK:63:ARG:N     | 2.75                     | 0.40              |
| 47:DO:2:ILE:HD11   | 47:DO:82:ASN:ND2   | 2.33                     | 0.40              |
| 47:DO:68:GLU:CB    | 47:DO:78:ARG:HB2   | 2.52                     | 0.40              |
| 47:DO:68:GLU:N     | 47:DO:68:GLU:OE2   | 2.54                     | 0.40              |
| 48:DP:13:ASN:ND2   | 48:DP:13:ASN:O     | 2.54                     | 0.40              |
| 33:D8:58:ILE:CG2   | 48:DP:49:ARG:HD3   | 2.52                     | 0.40              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 52:DT:78:LEU:HB3  | 52:DT:79:HIS:CE1  | 2.57                     | 0.40              |
| 35:DA:2012:G:O3'  | 55:DW:96:ILE:HG13 | 2.20                     | 0.40              |
| 56:DX:8:ILE:CD1   | 56:DX:42:ALA:O    | 2.69                     | 0.40              |
| 58:DZ:120:ILE:O   | 58:DZ:121:HIS:HB2 | 2.20                     | 0.40              |
| 58:DZ:29:TYR:CB   | 58:DZ:34:ASN:HB2  | 2.36                     | 0.40              |
| 1:AA:1109:C:C2'   | 1:AA:1110:A:H5'   | 2.51                     | 0.40              |
| 1:AA:1296:C:O2'   | 1:AA:1302:U:C5    | 2.63                     | 0.40              |
| 1:AA:1465:C:C2'   | 1:AA:1466:C:H5'   | 2.52                     | 0.40              |
| 1:AA:226:G:O2'    | 1:AA:227:G:H5'    | 2.22                     | 0.40              |
| 1:AA:262:A:C6     | 1:AA:263:A:C6     | 3.09                     | 0.40              |
| 1:AA:563:A:N7     | 1:AA:567:G:H1'    | 2.36                     | 0.40              |
| 1:AA:707:C:H2'    | 1:AA:708:C:C6     | 2.57                     | 0.40              |
| 1:AA:910:C:O2'    | 1:AA:911:U:H5'    | 2.22                     | 0.40              |
| 2:AB:194:PRO:O    | 2:AB:195:ASP:C    | 2.59                     | 0.40              |
| 2:AB:212:GLN:OE1  | 2:AB:216:SER:HB2  | 2.22                     | 0.40              |
| 4:AD:149:ALA:O    | 4:AD:153:ARG:HG3  | 2.22                     | 0.40              |
| 7:AG:61:VAL:O     | 7:AG:62:PHE:C     | 2.59                     | 0.40              |
| 1:AA:963:G:H21    | 10:AJ:55:LYS:HD2  | 1.86                     | 0.40              |
| 10:AJ:67:THR:HG22 | 10:AJ:67:THR:O    | 2.21                     | 0.40              |
| 10:AJ:61:GLU:HG3  | 14:AN:58:LYS:HE2  | 2.03                     | 0.40              |
| 16:AP:52:ASP:C    | 16:AP:52:ASP:OD2  | 2.58                     | 0.40              |
| 17:AQ:53:LEU:HD23 | 17:AQ:53:LEU:C    | 2.42                     | 0.40              |
| 6:AF:97:PHE:N     | 18:AR:30:ASP:OD1  | 2.51                     | 0.40              |
| 7:AG:77:SER:OG    | 22:AW:33:C:O3'    | 2.40                     | 0.40              |
| 24:AY:137:ASN:O   | 24:AY:262:SER:HA  | 2.21                     | 0.40              |
| 24:AY:152:THR:CG2 | 24:AY:153:MET:N   | 2.84                     | 0.40              |
| 24:AY:435:ASP:OD2 | 24:AY:437:THR:OG1 | 2.35                     | 0.40              |
| 24:AY:455:GLY:O   | 24:AY:456:GLU:C   | 2.59                     | 0.40              |
| 24:AY:554:PRO:HG2 | 24:AY:555:LEU:HG  | 2.04                     | 0.40              |
| 24:AY:616:TYR:O   | 24:AY:617:MET:C   | 2.60                     | 0.40              |
| 27:B2:29:LYS:O    | 27:B2:32:LEU:N    | 2.55                     | 0.40              |
| 30:B5:19:ARG:HA   | 35:BA:2046:G:H5'' | 2.01                     | 0.40              |
| 35:BA:1016:G:H1   | 35:BA:1146:C:H42  | 1.69                     | 0.40              |
| 35:BA:83:G:H22    | 35:BA:102:G:H2'   | 1.84                     | 0.40              |
| 35:BA:121:G:N2    | 35:BA:122:G:H1'   | 2.36                     | 0.40              |
| 35:BA:1337:G:H2'  | 35:BA:1338:G:H8   | 1.86                     | 0.40              |
| 26:B1:12:PRO:HG3  | 35:BA:1365:A:H5'  | 2.04                     | 0.40              |
| 35:BA:1398:C:H2'  | 35:BA:1399:C:C6   | 2.54                     | 0.40              |
| 35:BA:1459:G:O2'  | 35:BA:1461:G:H5'  | 2.22                     | 0.40              |
| 35:BA:1571:A:H8   | 35:BA:1571:A:O5'  | 2.04                     | 0.40              |
| 35:BA:2244:U:O5'  | 35:BA:2244:U:H6   | 2.04                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:BA:2078:C:H1'   | 35:BA:2434:A:H1'  | 2.04                     | 0.40              |
| 35:BA:2516:G:O2'   | 35:BA:2517:C:H5'  | 2.21                     | 0.40              |
| 35:BA:2579:C:H6    | 35:BA:2579:C:O5'  | 2.05                     | 0.40              |
| 35:BA:271(E):U:H2' | 35:BA:271(F):C:H6 | 1.85                     | 0.40              |
| 35:BA:2867:G:OP2   | 52:BT:119:LYS:NZ  | 2.54                     | 0.40              |
| 35:BA:572:A:H2'    | 35:BA:573:G:O4'   | 2.22                     | 0.40              |
| 35:BA:637:A:N6     | 35:BA:652:C:H4'   | 2.36                     | 0.40              |
| 35:BA:635:C:O2'    | 35:BA:639:U:OP1   | 2.38                     | 0.40              |
| 35:BA:777:A:C2     | 35:BA:778:G:C4    | 3.10                     | 0.40              |
| 35:BA:812:C:C2     | 35:BA:813:U:C5    | 3.09                     | 0.40              |
| 35:BA:910:A:C6     | 35:BA:911:A:C6    | 3.10                     | 0.40              |
| 36:BB:29:A:C2      | 36:BB:56:G:C2     | 3.10                     | 0.40              |
| 40:BF:157:VAL:CG2  | 40:BF:194:MET:HA  | 2.52                     | 0.40              |
| 40:BF:89:VAL:CG1   | 40:BF:90:PHE:H    | 2.27                     | 0.40              |
| 41:BG:106:LEU:HG   | 41:BG:106:LEU:O   | 2.20                     | 0.40              |
| 41:BG:34:LEU:HD11  | 41:BG:100:TRP:CZ2 | 2.55                     | 0.40              |
| 41:BG:37:VAL:HG22  | 41:BG:159:VAL:HB  | 2.03                     | 0.40              |
| 41:BG:44:GLY:O     | 41:BG:47:LYS:CD   | 2.70                     | 0.40              |
| 42:BH:19:VAL:O     | 42:BH:20:ALA:CB   | 2.69                     | 0.40              |
| 42:BH:41:MET:HE2   | 42:BH:43:VAL:HA   | 2.04                     | 0.40              |
| 44:BK:41:PHE:O     | 44:BK:43:ALA:N    | 2.54                     | 0.40              |
| 46:BN:40:PRO:O     | 53:BU:64:ARG:NH2  | 2.53                     | 0.40              |
| 48:BP:71:VAL:N     | 48:BP:72:PRO:CD   | 2.85                     | 0.40              |
| 48:BP:91:PHE:HZ    | 48:BP:100:LEU:CD1 | 2.32                     | 0.40              |
| 35:BA:1278:A:C5'   | 50:BR:36:THR:HG22 | 2.50                     | 0.40              |
| 52:BT:50:ILE:HD11  | 52:BT:64:ARG:HB3  | 2.03                     | 0.40              |
| 54:BV:32:THR:HG23  | 54:BV:60:GLU:HA   | 2.04                     | 0.40              |
| 57:BY:11:ASP:O     | 57:BY:27:VAL:HA   | 2.22                     | 0.40              |
| 58:BZ:127:LYS:HZ3  | 58:BZ:127:LYS:HB3 | 1.86                     | 0.40              |
| 58:BZ:162:GLU:O    | 58:BZ:163:LEU:C   | 2.60                     | 0.40              |
| 1:CA:267:C:H2'     | 1:CA:268:C:C6     | 2.47                     | 0.40              |
| 1:CA:301:G:H2'     | 1:CA:302:G:H8     | 1.87                     | 0.40              |
| 1:CA:313:A:H2'     | 1:CA:314:C:C6     | 2.57                     | 0.40              |
| 1:CA:407:G:H2'     | 1:CA:408:A:C8     | 2.54                     | 0.40              |
| 1:CA:436:C:O2'     | 1:CA:437:U:P      | 2.80                     | 0.40              |
| 1:CA:841:U:H3'     | 1:CA:848:C:H5'    | 2.04                     | 0.40              |
| 1:CA:977:A:HO2'    | 1:CA:978:A:H5'    | 1.87                     | 0.40              |
| 2:CB:121:LEU:HA    | 2:CB:124:SER:CB   | 2.50                     | 0.40              |
| 3:CC:9:GLY:HA2     | 3:CC:12:LEU:HG    | 2.04                     | 0.40              |
| 4:CD:159:ARG:O     | 4:CD:160:GLN:C    | 2.60                     | 0.40              |
| 4:CD:190:ASP:HB3   | 4:CD:193:ASP:OD2  | 2.22                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:CE:101:ILE:CD1   | 5:CE:118:ILE:O     | 2.67                     | 0.40              |
| 5:CE:128:PRO:O     | 5:CE:129:ILE:C     | 2.60                     | 0.40              |
| 6:CF:50:TYR:HB2    | 6:CF:51:PRO:HD2    | 2.03                     | 0.40              |
| 7:CG:134:ALA:O     | 7:CG:135:VAL:C     | 2.60                     | 0.40              |
| 8:CH:43:GLY:O      | 8:CH:64:LYS:NZ     | 2.42                     | 0.40              |
| 9:CI:4:TYR:CB      | 9:CI:19:LEU:HB2    | 2.22                     | 0.40              |
| 9:CI:16:ARG:O      | 9:CI:63:ILE:HG23   | 2.21                     | 0.40              |
| 10:CJ:22:LYS:C     | 10:CJ:24:VAL:H     | 2.25                     | 0.40              |
| 13:CM:40:ASN:HD21  | 13:CM:42:ALA:HB3   | 1.86                     | 0.40              |
| 13:CM:49:THR:C     | 13:CM:51:ALA:H     | 2.25                     | 0.40              |
| 15:CO:74:ASP:O     | 15:CO:76:GLU:N     | 2.53                     | 0.40              |
| 16:CP:60:LEU:HA    | 16:CP:60:LEU:HD23  | 1.94                     | 0.40              |
| 17:CQ:10:VAL:HG13  | 17:CQ:19:VAL:HB    | 2.03                     | 0.40              |
| 24:CY:128:TYR:CD1  | 24:CY:128:TYR:O    | 2.75                     | 0.40              |
| 24:CY:141:LYS:O    | 24:CY:144:ALA:HB2  | 2.22                     | 0.40              |
| 24:CY:345:THR:O    | 24:CY:345:THR:HG22 | 2.21                     | 0.40              |
| 24:CY:507:TYR:C    | 24:CY:507:TYR:HD1  | 2.22                     | 0.40              |
| 34:D9:19:ARG:O     | 34:D9:20:HIS:HB2   | 2.21                     | 0.40              |
| 34:D9:3:VAL:HG21   | 35:DA:2539:C:H4'   | 2.04                     | 0.40              |
| 35:DA:1010:A:H1'   | 35:DA:1153:C:C1'   | 2.49                     | 0.40              |
| 35:DA:1043:C:H6    | 35:DA:1043:C:O5'   | 2.05                     | 0.40              |
| 35:DA:1049:C:H6    | 35:DA:1049:C:H5'   | 1.86                     | 0.40              |
| 35:DA:2352:A:C2'   | 35:DA:2353:G:H5'   | 2.51                     | 0.40              |
| 35:DA:2393:A:H2'   | 35:DA:2394:C:O4'   | 2.22                     | 0.40              |
| 35:DA:2454:G:H2'   | 35:DA:2455:G:C5'   | 2.52                     | 0.40              |
| 35:DA:2652:C:H42   | 35:DA:2668:G:H1    | 1.70                     | 0.40              |
| 35:DA:271(P):C:H2' | 35:DA:271(Q):G:C8  | 2.56                     | 0.40              |
| 35:DA:312:G:H2'    | 35:DA:313:C:O4'    | 2.22                     | 0.40              |
| 35:DA:482:A:N6     | 35:DA:506:G:C8     | 2.89                     | 0.40              |
| 35:DA:772:C:O2'    | 35:DA:773:U:H5'    | 2.21                     | 0.40              |
| 35:DA:811:U:O2     | 35:DA:1251:C:C6    | 2.75                     | 0.40              |
| 35:DA:999:U:O2     | 35:DA:1157:G:C2    | 2.75                     | 0.40              |
| 37:DC:172:ILE:HG21 | 37:DC:197:LEU:HD11 | 2.03                     | 0.40              |
| 35:DA:2821:A:OP2   | 39:DE:110:GLY:O    | 2.39                     | 0.40              |
| 39:DE:167:VAL:HG13 | 39:DE:170:LEU:HD11 | 2.03                     | 0.40              |
| 40:DF:157:VAL:HA   | 40:DF:176:LEU:O    | 2.21                     | 0.40              |
| 42:DH:28:GLY:HA3   | 42:DH:79:VAL:HG21  | 2.02                     | 0.40              |
| 43:DJ:69:UNK:O     | 43:DJ:70:UNK:O     | 2.40                     | 0.40              |
| 44:DK:30:HIS:CE1   | 44:DK:59:ILE:HB    | 2.56                     | 0.40              |
| 44:DK:6:ALA:HB3    | 44:DK:59:ILE:HG22  | 2.03                     | 0.40              |
| 47:DO:114:ILE:O    | 47:DO:117:LEU:N    | 2.45                     | 0.40              |

*Continued on next page...*

Continued from previous page...

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 35:DA:626:U:N3    | 48:DP:105:LEU:HG | 2.36                     | 0.40              |
| 35:DA:1453:U:OP1  | 50:DR:63:ARG:NH2 | 2.54                     | 0.40              |
| 50:DR:88:ARG:HD2  | 50:DR:88:ARG:O   | 2.21                     | 0.40              |
| 1:CA:1442(B):A:C5 | 52:DT:118:ARG:NE | 2.89                     | 0.40              |
| 53:DU:104:GLN:HB3 | 54:DV:44:LYS:HZ3 | 1.87                     | 0.40              |
| 53:DU:33:ARG:C    | 53:DU:35:ALA:H   | 2.25                     | 0.40              |
| 35:DA:2019:A:C4'  | 53:DU:34:LYS:HD2 | 2.51                     | 0.40              |
| 54:DV:19:LYS:HG2  | 54:DV:94:LEU:CB  | 2.47                     | 0.40              |
| 54:DV:32:THR:HG23 | 54:DV:60:GLU:HA  | 2.04                     | 0.40              |
| 58:DZ:129:SER:HB2 | 58:DZ:131:ARG:CD | 2.52                     | 0.40              |
| 58:DZ:35:ARG:NH1  | 58:DZ:35:ARG:CG  | 2.82                     | 0.40              |

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1        | Atom-2                  | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|-------------------------|--------------------------|-------------------|
| 2:CB:65:GLY:O | 37:DC:28:ARG:NH2[2_646] | 1.56                     | 0.64              |
| 2:CB:65:GLY:O | 37:DC:28:ARG:CZ[2_646]  | 1.87                     | 0.33              |

## 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   | AB    | 233/256 (91%) | 139 (60%) | 53 (23%) | 41 (18%) | 0           | 3  |
| 2   | CB    | 233/256 (91%) | 140 (60%) | 51 (22%) | 42 (18%) | 0           | 3  |
| 3   | AC    | 205/239 (86%) | 133 (65%) | 50 (24%) | 22 (11%) | 0           | 9  |
| 3   | CC    | 205/239 (86%) | 132 (64%) | 52 (25%) | 21 (10%) | 1           | 10 |
| 4   | AD    | 206/209 (99%) | 134 (65%) | 50 (24%) | 22 (11%) | 0           | 9  |
| 4   | CD    | 206/209 (99%) | 134 (65%) | 51 (25%) | 21 (10%) | 1           | 10 |
| 5   | AE    | 149/162 (92%) | 119 (80%) | 21 (14%) | 9 (6%)   | 2           | 22 |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 5   | CE    | 149/162 (92%) | 117 (78%) | 24 (16%) | 8 (5%)   | 2           | 24 |
| 6   | AF    | 99/101 (98%)  | 75 (76%)  | 17 (17%) | 7 (7%)   | 1           | 18 |
| 6   | CF    | 99/101 (98%)  | 74 (75%)  | 18 (18%) | 7 (7%)   | 1           | 18 |
| 7   | AG    | 153/156 (98%) | 109 (71%) | 34 (22%) | 10 (6%)  | 1           | 21 |
| 7   | CG    | 153/156 (98%) | 110 (72%) | 32 (21%) | 11 (7%)  | 1           | 17 |
| 8   | AH    | 136/138 (99%) | 103 (76%) | 30 (22%) | 3 (2%)   | 8           | 47 |
| 8   | CH    | 136/138 (99%) | 105 (77%) | 27 (20%) | 4 (3%)   | 5           | 41 |
| 9   | AI    | 121/128 (94%) | 81 (67%)  | 26 (22%) | 14 (12%) | 0           | 7  |
| 9   | CI    | 121/128 (94%) | 82 (68%)  | 27 (22%) | 12 (10%) | 1           | 10 |
| 10  | AJ    | 97/105 (92%)  | 60 (62%)  | 21 (22%) | 16 (16%) | 0           | 4  |
| 10  | CJ    | 97/105 (92%)  | 61 (63%)  | 20 (21%) | 16 (16%) | 0           | 4  |
| 11  | AK    | 117/129 (91%) | 91 (78%)  | 20 (17%) | 6 (5%)   | 2           | 26 |
| 11  | CK    | 117/129 (91%) | 91 (78%)  | 20 (17%) | 6 (5%)   | 2           | 26 |
| 12  | AL    | 123/132 (93%) | 82 (67%)  | 23 (19%) | 18 (15%) | 0           | 5  |
| 12  | CL    | 123/132 (93%) | 82 (67%)  | 22 (18%) | 19 (15%) | 0           | 4  |
| 13  | AM    | 123/126 (98%) | 77 (63%)  | 25 (20%) | 21 (17%) | 0           | 3  |
| 13  | CM    | 123/126 (98%) | 77 (63%)  | 26 (21%) | 20 (16%) | 0           | 4  |
| 14  | AN    | 58/61 (95%)   | 47 (81%)  | 7 (12%)  | 4 (7%)   | 1           | 19 |
| 14  | CN    | 58/61 (95%)   | 46 (79%)  | 7 (12%)  | 5 (9%)   | 1           | 13 |
| 15  | AO    | 86/89 (97%)   | 55 (64%)  | 23 (27%) | 8 (9%)   | 1           | 11 |
| 15  | CO    | 86/89 (97%)   | 53 (62%)  | 24 (28%) | 9 (10%)  | 0           | 9  |
| 16  | AP    | 82/88 (93%)   | 60 (73%)  | 15 (18%) | 7 (8%)   | 1           | 13 |
| 16  | CP    | 82/88 (93%)   | 60 (73%)  | 15 (18%) | 7 (8%)   | 1           | 13 |
| 17  | AQ    | 98/105 (93%)  | 78 (80%)  | 15 (15%) | 5 (5%)   | 2           | 26 |
| 17  | CQ    | 98/105 (93%)  | 78 (80%)  | 16 (16%) | 4 (4%)   | 3           | 32 |
| 18  | AR    | 68/88 (77%)   | 52 (76%)  | 11 (16%) | 5 (7%)   | 1           | 16 |
| 18  | CR    | 68/88 (77%)   | 51 (75%)  | 12 (18%) | 5 (7%)   | 1           | 16 |
| 19  | AS    | 77/93 (83%)   | 43 (56%)  | 14 (18%) | 20 (26%) | 0           | 1  |
| 19  | CS    | 77/93 (83%)   | 43 (56%)  | 15 (20%) | 19 (25%) | 0           | 1  |
| 20  | AT    | 97/106 (92%)  | 52 (54%)  | 30 (31%) | 15 (16%) | 0           | 4  |
| 20  | CT    | 97/106 (92%)  | 53 (55%)  | 29 (30%) | 15 (16%) | 0           | 4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed      | Favoured  | Allowed   | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|-----------|----------|-------------|----|
| 21  | AU    | 23/27 (85%)   | 14 (61%)  | 6 (26%)   | 3 (13%)  | 0           | 6  |
| 21  | CU    | 23/27 (85%)   | 14 (61%)  | 5 (22%)   | 4 (17%)  | 0           | 3  |
| 24  | AY    | 663/691 (96%) | 435 (66%) | 137 (21%) | 91 (14%) | 0           | 5  |
| 24  | CY    | 663/691 (96%) | 449 (68%) | 134 (20%) | 80 (12%) | 0           | 7  |
| 25  | B0    | 82/85 (96%)   | 64 (78%)  | 14 (17%)  | 4 (5%)   | 2           | 27 |
| 25  | D0    | 82/85 (96%)   | 64 (78%)  | 14 (17%)  | 4 (5%)   | 2           | 27 |
| 26  | B1    | 92/98 (94%)   | 64 (70%)  | 15 (16%)  | 13 (14%) | 0           | 5  |
| 26  | D1    | 92/98 (94%)   | 67 (73%)  | 13 (14%)  | 12 (13%) | 0           | 6  |
| 27  | B2    | 69/72 (96%)   | 35 (51%)  | 18 (26%)  | 16 (23%) | 0           | 1  |
| 27  | D2    | 69/72 (96%)   | 29 (42%)  | 31 (45%)  | 9 (13%)  | 0           | 6  |
| 28  | B3    | 58/60 (97%)   | 41 (71%)  | 12 (21%)  | 5 (9%)   | 1           | 13 |
| 28  | D3    | 58/60 (97%)   | 41 (71%)  | 12 (21%)  | 5 (9%)   | 1           | 13 |
| 29  | B4    | 56/71 (79%)   | 27 (48%)  | 14 (25%)  | 15 (27%) | 0           | 0  |
| 29  | D4    | 56/71 (79%)   | 28 (50%)  | 13 (23%)  | 15 (27%) | 0           | 0  |
| 30  | B5    | 57/60 (95%)   | 37 (65%)  | 9 (16%)   | 11 (19%) | 0           | 2  |
| 30  | D5    | 57/60 (95%)   | 38 (67%)  | 7 (12%)   | 12 (21%) | 0           | 2  |
| 31  | B6    | 48/54 (89%)   | 21 (44%)  | 12 (25%)  | 15 (31%) | 0           | 0  |
| 31  | D6    | 48/54 (89%)   | 22 (46%)  | 12 (25%)  | 14 (29%) | 0           | 0  |
| 32  | B7    | 47/49 (96%)   | 35 (74%)  | 11 (23%)  | 1 (2%)   | 8           | 48 |
| 32  | D7    | 47/49 (96%)   | 35 (74%)  | 11 (23%)  | 1 (2%)   | 8           | 48 |
| 33  | B8    | 62/65 (95%)   | 34 (55%)  | 16 (26%)  | 12 (19%) | 0           | 2  |
| 33  | D8    | 62/65 (95%)   | 34 (55%)  | 16 (26%)  | 12 (19%) | 0           | 2  |
| 34  | B9    | 35/37 (95%)   | 21 (60%)  | 9 (26%)   | 5 (14%)  | 0           | 5  |
| 34  | D9    | 35/37 (95%)   | 21 (60%)  | 8 (23%)   | 6 (17%)  | 0           | 3  |
| 37  | BC    | 226/229 (99%) | 163 (72%) | 51 (23%)  | 12 (5%)  | 2           | 25 |
| 37  | DC    | 226/229 (99%) | 163 (72%) | 50 (22%)  | 13 (6%)  | 2           | 23 |
| 38  | BD    | 273/276 (99%) | 189 (69%) | 50 (18%)  | 34 (12%) | 0           | 7  |
| 38  | DD    | 273/276 (99%) | 188 (69%) | 50 (18%)  | 35 (13%) | 0           | 6  |
| 39  | BE    | 203/206 (98%) | 122 (60%) | 45 (22%)  | 36 (18%) | 0           | 3  |
| 39  | DE    | 203/206 (98%) | 124 (61%) | 44 (22%)  | 35 (17%) | 0           | 3  |
| 40  | BF    | 206/210 (98%) | 132 (64%) | 44 (21%)  | 30 (15%) | 0           | 5  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 40  | DF    | 206/210 (98%) | 133 (65%) | 42 (20%) | 31 (15%) | 0           | 4  |
| 41  | BG    | 177/182 (97%) | 110 (62%) | 43 (24%) | 24 (14%) | 0           | 5  |
| 41  | DG    | 177/182 (97%) | 115 (65%) | 36 (20%) | 26 (15%) | 0           | 5  |
| 42  | BH    | 165/180 (92%) | 86 (52%)  | 40 (24%) | 39 (24%) | 0           | 1  |
| 42  | DH    | 165/180 (92%) | 86 (52%)  | 40 (24%) | 39 (24%) | 0           | 1  |
| 44  | BK    | 138/147 (94%) | 92 (67%)  | 35 (25%) | 11 (8%)  | 1           | 14 |
| 44  | DK    | 138/147 (94%) | 92 (67%)  | 35 (25%) | 11 (8%)  | 1           | 14 |
| 46  | BN    | 137/140 (98%) | 88 (64%)  | 28 (20%) | 21 (15%) | 0           | 4  |
| 46  | DN    | 137/140 (98%) | 88 (64%)  | 28 (20%) | 21 (15%) | 0           | 4  |
| 47  | BO    | 120/122 (98%) | 91 (76%)  | 19 (16%) | 10 (8%)  | 1           | 13 |
| 47  | DO    | 120/122 (98%) | 93 (78%)  | 17 (14%) | 10 (8%)  | 1           | 13 |
| 48  | BP    | 144/150 (96%) | 72 (50%)  | 45 (31%) | 27 (19%) | 0           | 2  |
| 48  | DP    | 144/150 (96%) | 72 (50%)  | 44 (31%) | 28 (19%) | 0           | 2  |
| 49  | BQ    | 139/141 (99%) | 106 (76%) | 26 (19%) | 7 (5%)   | 2           | 26 |
| 49  | DQ    | 139/141 (99%) | 106 (76%) | 26 (19%) | 7 (5%)   | 2           | 26 |
| 50  | BR    | 115/118 (98%) | 81 (70%)  | 20 (17%) | 14 (12%) | 0           | 7  |
| 50  | DR    | 115/118 (98%) | 81 (70%)  | 20 (17%) | 14 (12%) | 0           | 7  |
| 51  | BS    | 97/112 (87%)  | 41 (42%)  | 35 (36%) | 21 (22%) | 0           | 1  |
| 51  | DS    | 97/112 (87%)  | 41 (42%)  | 35 (36%) | 21 (22%) | 0           | 1  |
| 52  | BT    | 136/146 (93%) | 76 (56%)  | 32 (24%) | 28 (21%) | 0           | 2  |
| 52  | DT    | 136/146 (93%) | 75 (55%)  | 32 (24%) | 29 (21%) | 0           | 2  |
| 53  | BU    | 115/118 (98%) | 66 (57%)  | 37 (32%) | 12 (10%) | 0           | 10 |
| 53  | DU    | 115/118 (98%) | 67 (58%)  | 35 (30%) | 13 (11%) | 0           | 8  |
| 54  | BV    | 99/101 (98%)  | 69 (70%)  | 12 (12%) | 18 (18%) | 0           | 2  |
| 54  | DV    | 99/101 (98%)  | 69 (70%)  | 12 (12%) | 18 (18%) | 0           | 2  |
| 55  | BW    | 111/113 (98%) | 80 (72%)  | 21 (19%) | 10 (9%)  | 1           | 12 |
| 55  | DW    | 111/113 (98%) | 81 (73%)  | 21 (19%) | 9 (8%)   | 1           | 14 |
| 56  | BX    | 91/96 (95%)   | 56 (62%)  | 26 (29%) | 9 (10%)  | 1           | 10 |
| 56  | DX    | 91/96 (95%)   | 57 (63%)  | 25 (28%) | 9 (10%)  | 1           | 10 |
| 57  | BY    | 105/110 (96%) | 42 (40%)  | 36 (34%) | 27 (26%) | 0           | 1  |
| 57  | DY    | 105/110 (96%) | 43 (41%)  | 36 (34%) | 26 (25%) | 0           | 1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed          | Favoured   | Allowed    | Outliers   | Percentiles |   |
|-----|-------|-------------------|------------|------------|------------|-------------|---|
| 58  | BZ    | 183/206 (89%)     | 108 (59%)  | 42 (23%)   | 33 (18%)   | 0           | 3 |
| 58  | DZ    | 183/206 (89%)     | 114 (62%)  | 37 (20%)   | 32 (18%)   | 0           | 3 |
| All | All   | 13200/13966 (94%) | 8607 (65%) | 2874 (22%) | 1719 (13%) | 0           | 6 |

All (1719) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 12  | GLU  |
| 2   | AB    | 13  | ALA  |
| 2   | AB    | 15  | VAL  |
| 2   | AB    | 20  | GLU  |
| 2   | AB    | 95  | GLN  |
| 2   | AB    | 129 | GLU  |
| 2   | AB    | 190 | THR  |
| 2   | AB    | 195 | ASP  |
| 2   | AB    | 233 | SER  |
| 2   | AB    | 239 | VAL  |
| 3   | AC    | 12  | LEU  |
| 3   | AC    | 47  | LEU  |
| 3   | AC    | 61  | ALA  |
| 3   | AC    | 95  | THR  |
| 3   | AC    | 154 | SER  |
| 3   | AC    | 156 | ARG  |
| 3   | AC    | 207 | VAL  |
| 4   | AD    | 3   | ARG  |
| 4   | AD    | 13  | ARG  |
| 4   | AD    | 14  | ARG  |
| 4   | AD    | 18  | LYS  |
| 4   | AD    | 30  | LYS  |
| 4   | AD    | 32  | ALA  |
| 4   | AD    | 44  | GLY  |
| 4   | AD    | 153 | ARG  |
| 4   | AD    | 179 | GLU  |
| 5   | AE    | 11  | ILE  |
| 6   | AF    | 39  | LYS  |
| 7   | AG    | 8   | GLU  |
| 7   | AG    | 52  | GLU  |
| 7   | AG    | 90  | GLU  |
| 8   | AH    | 105 | ARG  |
| 9   | AI    | 41  | VAL  |
| 9   | AI    | 43  | ALA  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | AI    | 61  | ALA  |
| 9   | AI    | 89  | ASN  |
| 10  | AJ    | 33  | GLN  |
| 10  | AJ    | 36  | GLY  |
| 10  | AJ    | 55  | LYS  |
| 10  | AJ    | 56  | HIS  |
| 10  | AJ    | 57  | LYS  |
| 10  | AJ    | 59  | SER  |
| 10  | AJ    | 75  | ILE  |
| 11  | AK    | 123 | LYS  |
| 11  | AK    | 127 | LYS  |
| 12  | AL    | 18  | VAL  |
| 12  | AL    | 27  | LEU  |
| 12  | AL    | 28  | LYS  |
| 12  | AL    | 38  | THR  |
| 12  | AL    | 45  | PRO  |
| 12  | AL    | 81  | SER  |
| 12  | AL    | 91  | LYS  |
| 13  | AM    | 12  | ASN  |
| 13  | AM    | 67  | GLU  |
| 13  | AM    | 70  | LEU  |
| 13  | AM    | 83  | ASP  |
| 13  | AM    | 90  | LEU  |
| 13  | AM    | 91  | ARG  |
| 13  | AM    | 100 | GLY  |
| 13  | AM    | 118 | ALA  |
| 13  | AM    | 124 | PRO  |
| 14  | AN    | 15  | LYS  |
| 14  | AN    | 29  | ARG  |
| 15  | AO    | 24  | SER  |
| 16  | AP    | 83  | GLU  |
| 17  | AQ    | 13  | ASP  |
| 17  | AQ    | 49  | GLU  |
| 18  | AR    | 37  | VAL  |
| 18  | AR    | 38  | GLU  |
| 18  | AR    | 45  | SER  |
| 19  | AS    | 10  | PHE  |
| 19  | AS    | 27  | GLU  |
| 19  | AS    | 28  | LYS  |
| 19  | AS    | 29  | ARG  |
| 19  | AS    | 47  | HIS  |
| 19  | AS    | 61  | TYR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | AT    | 48  | LYS  |
| 20  | AT    | 74  | LYS  |
| 20  | AT    | 99  | LEU  |
| 21  | AU    | 3   | LYS  |
| 24  | AY    | 6   | GLU  |
| 24  | AY    | 19  | ALA  |
| 24  | AY    | 21  | ILE  |
| 24  | AY    | 23  | ALA  |
| 24  | AY    | 66  | THR  |
| 24  | AY    | 68  | ALA  |
| 24  | AY    | 84  | THR  |
| 24  | AY    | 85  | PRO  |
| 24  | AY    | 88  | VAL  |
| 24  | AY    | 92  | ILE  |
| 24  | AY    | 119 | GLU  |
| 24  | AY    | 121 | VAL  |
| 24  | AY    | 129 | LYS  |
| 24  | AY    | 197 | ARG  |
| 24  | AY    | 203 | GLU  |
| 24  | AY    | 204 | GLU  |
| 24  | AY    | 205 | TYR  |
| 24  | AY    | 206 | LEU  |
| 24  | AY    | 209 | ALA  |
| 24  | AY    | 210 | ARG  |
| 24  | AY    | 251 | ILE  |
| 24  | AY    | 276 | VAL  |
| 24  | AY    | 360 | ALA  |
| 24  | AY    | 385 | THR  |
| 24  | AY    | 396 | ARG  |
| 24  | AY    | 402 | ILE  |
| 24  | AY    | 447 | GLY  |
| 24  | AY    | 448 | GLN  |
| 24  | AY    | 456 | GLU  |
| 24  | AY    | 498 | ILE  |
| 24  | AY    | 519 | ARG  |
| 24  | AY    | 530 | VAL  |
| 24  | AY    | 559 | PRO  |
| 24  | AY    | 614 | GLU  |
| 25  | B0    | 74  | ARG  |
| 26  | B1    | 28  | GLY  |
| 26  | B1    | 52  | ARG  |
| 26  | B1    | 53  | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | B1    | 85  | LEU  |
| 27  | B2    | 18  | PRO  |
| 27  | B2    | 19  | VAL  |
| 27  | B2    | 20  | GLU  |
| 27  | B2    | 47  | ASN  |
| 27  | B2    | 48  | HIS  |
| 28  | B3    | 3   | ARG  |
| 29  | B4    | 3   | GLU  |
| 29  | B4    | 26  | SER  |
| 29  | B4    | 38  | LYS  |
| 29  | B4    | 43  | TYR  |
| 29  | B4    | 50  | VAL  |
| 29  | B4    | 57  | GLU  |
| 30  | B5    | 49  | CYS  |
| 30  | B5    | 53  | ALA  |
| 30  | B5    | 56  | LYS  |
| 30  | B5    | 57  | VAL  |
| 31  | B6    | 7   | ILE  |
| 31  | B6    | 9   | LEU  |
| 31  | B6    | 18  | ARG  |
| 31  | B6    | 20  | ASN  |
| 31  | B6    | 27  | LYS  |
| 31  | B6    | 31  | PRO  |
| 31  | B6    | 44  | ARG  |
| 31  | B6    | 52  | VAL  |
| 33  | B8    | 31  | HIS  |
| 33  | B8    | 33  | ASN  |
| 33  | B8    | 43  | GLN  |
| 33  | B8    | 49  | VAL  |
| 34  | B9    | 2   | LYS  |
| 34  | B9    | 35  | ARG  |
| 38  | BD    | 19  | ALA  |
| 38  | BD    | 24  | ILE  |
| 38  | BD    | 25  | THR  |
| 38  | BD    | 27  | THR  |
| 38  | BD    | 30  | GLU  |
| 38  | BD    | 34  | VAL  |
| 38  | BD    | 35  | LYS  |
| 38  | BD    | 127 | VAL  |
| 38  | BD    | 225 | ALA  |
| 38  | BD    | 239 | ARG  |
| 38  | BD    | 246 | PRO  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | BE    | 35  | GLN  |
| 39  | BE    | 54  | GLN  |
| 39  | BE    | 77  | ILE  |
| 39  | BE    | 88  | GLY  |
| 39  | BE    | 90  | THR  |
| 39  | BE    | 145 | LYS  |
| 39  | BE    | 185 | LYS  |
| 39  | BE    | 189 | PRO  |
| 40  | BF    | 11  | VAL  |
| 40  | BF    | 21  | ALA  |
| 40  | BF    | 64  | ILE  |
| 40  | BF    | 89  | VAL  |
| 40  | BF    | 167 | ALA  |
| 41  | BG    | 4   | ASP  |
| 41  | BG    | 6   | ALA  |
| 41  | BG    | 47  | LYS  |
| 41  | BG    | 87  | PRO  |
| 41  | BG    | 96  | ARG  |
| 41  | BG    | 102 | PHE  |
| 41  | BG    | 109 | VAL  |
| 41  | BG    | 110 | ALA  |
| 41  | BG    | 181 | ARG  |
| 42  | BH    | 13  | LYS  |
| 42  | BH    | 20  | ALA  |
| 42  | BH    | 41  | MET  |
| 42  | BH    | 46  | GLU  |
| 42  | BH    | 55  | PRO  |
| 42  | BH    | 83  | TYR  |
| 42  | BH    | 154 | PRO  |
| 42  | BH    | 155 | SER  |
| 42  | BH    | 156 | ALA  |
| 42  | BH    | 157 | TYR  |
| 42  | BH    | 160 | LYS  |
| 42  | BH    | 169 | VAL  |
| 42  | BH    | 173 | PRO  |
| 44  | BK    | 51  | ALA  |
| 44  | BK    | 115 | LEU  |
| 46  | BN    | 8   | GLN  |
| 46  | BN    | 36  | GLY  |
| 46  | BN    | 46  | VAL  |
| 46  | BN    | 47  | ALA  |
| 46  | BN    | 57  | ALA  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | BN    | 58  | ASP  |
| 46  | BN    | 63  | THR  |
| 46  | BN    | 130 | HIS  |
| 46  | BN    | 133 | GLN  |
| 47  | BO    | 35  | VAL  |
| 47  | BO    | 48  | PRO  |
| 47  | BO    | 54  | GLU  |
| 47  | BO    | 68  | GLU  |
| 48  | BP    | 12  | ALA  |
| 48  | BP    | 14  | LYS  |
| 48  | BP    | 17  | LYS  |
| 48  | BP    | 31  | ALA  |
| 48  | BP    | 47  | ASP  |
| 48  | BP    | 48  | PRO  |
| 48  | BP    | 52  | GLU  |
| 48  | BP    | 57  | THR  |
| 48  | BP    | 58  | THR  |
| 48  | BP    | 111 | ARG  |
| 48  | BP    | 135 | LEU  |
| 48  | BP    | 147 | LEU  |
| 49  | BQ    | 27  | VAL  |
| 49  | BQ    | 135 | ASP  |
| 50  | BR    | 8   | ARG  |
| 50  | BR    | 14  | SER  |
| 50  | BR    | 58  | GLY  |
| 50  | BR    | 88  | ARG  |
| 50  | BR    | 107 | ASP  |
| 50  | BR    | 117 | VAL  |
| 51  | BS    | 13  | ARG  |
| 51  | BS    | 23  | ARG  |
| 51  | BS    | 97  | ARG  |
| 51  | BS    | 100 | ALA  |
| 51  | BS    | 102 | ALA  |
| 51  | BS    | 103 | GLU  |
| 52  | BT    | 5   | ALA  |
| 52  | BT    | 6   | LEU  |
| 52  | BT    | 24  | PRO  |
| 52  | BT    | 28  | VAL  |
| 52  | BT    | 30  | VAL  |
| 52  | BT    | 55  | ASN  |
| 52  | BT    | 80  | SER  |
| 52  | BT    | 91  | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52  | BT    | 104 | ASN  |
| 52  | BT    | 107 | ASP  |
| 52  | BT    | 130 | ALA  |
| 52  | BT    | 132 | LYS  |
| 52  | BT    | 135 | ALA  |
| 53  | BU    | 91  | ASP  |
| 53  | BU    | 93  | LYS  |
| 54  | BV    | 16  | PRO  |
| 54  | BV    | 18  | LEU  |
| 54  | BV    | 19  | LYS  |
| 54  | BV    | 46  | VAL  |
| 54  | BV    | 67  | GLY  |
| 55  | BW    | 63  | ASP  |
| 56  | BX    | 12  | VAL  |
| 56  | BX    | 42  | ALA  |
| 57  | BY    | 7   | VAL  |
| 57  | BY    | 24  | VAL  |
| 57  | BY    | 48  | ALA  |
| 57  | BY    | 60  | PHE  |
| 57  | BY    | 74  | PRO  |
| 57  | BY    | 77  | PRO  |
| 57  | BY    | 78  | ALA  |
| 57  | BY    | 99  | CYS  |
| 57  | BY    | 100 | ALA  |
| 57  | BY    | 104 | GLY  |
| 58  | BZ    | 27  | VAL  |
| 58  | BZ    | 51  | ALA  |
| 58  | BZ    | 78  | LYS  |
| 58  | BZ    | 80  | ARG  |
| 58  | BZ    | 81  | ARG  |
| 58  | BZ    | 120 | ILE  |
| 58  | BZ    | 121 | HIS  |
| 58  | BZ    | 142 | SER  |
| 58  | BZ    | 146 | ILE  |
| 58  | BZ    | 152 | ALA  |
| 58  | BZ    | 163 | LEU  |
| 58  | BZ    | 168 | GLU  |
| 58  | BZ    | 185 | GLU  |
| 58  | BZ    | 186 | GLU  |
| 2   | CB    | 12  | GLU  |
| 2   | CB    | 13  | ALA  |
| 2   | CB    | 15  | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | CB    | 20  | GLU  |
| 2   | CB    | 95  | GLN  |
| 2   | CB    | 129 | GLU  |
| 2   | CB    | 195 | ASP  |
| 2   | CB    | 233 | SER  |
| 2   | CB    | 239 | VAL  |
| 3   | CC    | 12  | LEU  |
| 3   | CC    | 47  | LEU  |
| 3   | CC    | 61  | ALA  |
| 3   | CC    | 95  | THR  |
| 3   | CC    | 154 | SER  |
| 3   | CC    | 156 | ARG  |
| 3   | CC    | 207 | VAL  |
| 4   | CD    | 3   | ARG  |
| 4   | CD    | 13  | ARG  |
| 4   | CD    | 14  | ARG  |
| 4   | CD    | 18  | LYS  |
| 4   | CD    | 30  | LYS  |
| 4   | CD    | 32  | ALA  |
| 4   | CD    | 44  | GLY  |
| 4   | CD    | 153 | ARG  |
| 4   | CD    | 171 | GLY  |
| 5   | CE    | 11  | ILE  |
| 6   | CF    | 39  | LYS  |
| 7   | CG    | 8   | GLU  |
| 7   | CG    | 52  | GLU  |
| 7   | CG    | 90  | GLU  |
| 8   | CH    | 105 | ARG  |
| 9   | CI    | 41  | VAL  |
| 9   | CI    | 43  | ALA  |
| 9   | CI    | 61  | ALA  |
| 9   | CI    | 89  | ASN  |
| 10  | CJ    | 33  | GLN  |
| 10  | CJ    | 36  | GLY  |
| 10  | CJ    | 55  | LYS  |
| 10  | CJ    | 56  | HIS  |
| 10  | CJ    | 57  | LYS  |
| 10  | CJ    | 59  | SER  |
| 10  | CJ    | 75  | ILE  |
| 11  | CK    | 123 | LYS  |
| 11  | CK    | 127 | LYS  |
| 12  | CL    | 18  | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | CL    | 27  | LEU  |
| 12  | CL    | 28  | LYS  |
| 12  | CL    | 38  | THR  |
| 12  | CL    | 45  | PRO  |
| 12  | CL    | 81  | SER  |
| 12  | CL    | 91  | LYS  |
| 13  | CM    | 12  | ASN  |
| 13  | CM    | 67  | GLU  |
| 13  | CM    | 70  | LEU  |
| 13  | CM    | 83  | ASP  |
| 13  | CM    | 90  | LEU  |
| 13  | CM    | 91  | ARG  |
| 13  | CM    | 100 | GLY  |
| 13  | CM    | 118 | ALA  |
| 13  | CM    | 124 | PRO  |
| 14  | CN    | 15  | LYS  |
| 14  | CN    | 29  | ARG  |
| 15  | CO    | 24  | SER  |
| 16  | CP    | 83  | GLU  |
| 17  | CQ    | 13  | ASP  |
| 17  | CQ    | 49  | GLU  |
| 18  | CR    | 37  | VAL  |
| 18  | CR    | 38  | GLU  |
| 18  | CR    | 45  | SER  |
| 19  | CS    | 10  | PHE  |
| 19  | CS    | 27  | GLU  |
| 19  | CS    | 28  | LYS  |
| 19  | CS    | 29  | ARG  |
| 19  | CS    | 47  | HIS  |
| 19  | CS    | 61  | TYR  |
| 20  | CT    | 48  | LYS  |
| 20  | CT    | 74  | LYS  |
| 20  | CT    | 99  | LEU  |
| 21  | CU    | 3   | LYS  |
| 24  | CY    | 21  | ILE  |
| 24  | CY    | 39  | ILE  |
| 24  | CY    | 66  | THR  |
| 24  | CY    | 67  | ALA  |
| 24  | CY    | 84  | THR  |
| 24  | CY    | 92  | ILE  |
| 24  | CY    | 104 | ALA  |
| 24  | CY    | 138 | LYS  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | CY    | 183 | MET  |
| 24  | CY    | 209 | ALA  |
| 24  | CY    | 210 | ARG  |
| 24  | CY    | 297 | GLU  |
| 24  | CY    | 299 | VAL  |
| 24  | CY    | 448 | GLN  |
| 24  | CY    | 456 | GLU  |
| 24  | CY    | 498 | ILE  |
| 24  | CY    | 530 | VAL  |
| 24  | CY    | 674 | ASP  |
| 25  | D0    | 74  | ARG  |
| 26  | D1    | 53  | VAL  |
| 27  | D2    | 47  | ASN  |
| 27  | D2    | 48  | HIS  |
| 28  | D3    | 3   | ARG  |
| 29  | D4    | 26  | SER  |
| 29  | D4    | 38  | LYS  |
| 29  | D4    | 43  | TYR  |
| 29  | D4    | 50  | VAL  |
| 29  | D4    | 57  | GLU  |
| 30  | D5    | 49  | CYS  |
| 30  | D5    | 53  | ALA  |
| 30  | D5    | 56  | LYS  |
| 30  | D5    | 57  | VAL  |
| 31  | D6    | 7   | ILE  |
| 31  | D6    | 9   | LEU  |
| 31  | D6    | 18  | ARG  |
| 31  | D6    | 20  | ASN  |
| 31  | D6    | 27  | LYS  |
| 31  | D6    | 31  | PRO  |
| 31  | D6    | 44  | ARG  |
| 31  | D6    | 52  | VAL  |
| 33  | D8    | 31  | HIS  |
| 33  | D8    | 33  | ASN  |
| 33  | D8    | 43  | GLN  |
| 33  | D8    | 49  | VAL  |
| 34  | D9    | 2   | LYS  |
| 34  | D9    | 35  | ARG  |
| 38  | DD    | 19  | ALA  |
| 38  | DD    | 24  | ILE  |
| 38  | DD    | 25  | THR  |
| 38  | DD    | 27  | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | DD    | 34  | VAL  |
| 38  | DD    | 35  | LYS  |
| 38  | DD    | 127 | VAL  |
| 38  | DD    | 225 | ALA  |
| 38  | DD    | 239 | ARG  |
| 38  | DD    | 246 | PRO  |
| 39  | DE    | 35  | GLN  |
| 39  | DE    | 54  | GLN  |
| 39  | DE    | 77  | ILE  |
| 39  | DE    | 88  | GLY  |
| 39  | DE    | 90  | THR  |
| 39  | DE    | 145 | LYS  |
| 39  | DE    | 185 | LYS  |
| 39  | DE    | 189 | PRO  |
| 40  | DF    | 11  | VAL  |
| 40  | DF    | 21  | ALA  |
| 40  | DF    | 64  | ILE  |
| 40  | DF    | 89  | VAL  |
| 40  | DF    | 167 | ALA  |
| 41  | DG    | 4   | ASP  |
| 41  | DG    | 14  | GLU  |
| 41  | DG    | 47  | LYS  |
| 41  | DG    | 48  | GLU  |
| 41  | DG    | 75  | LYS  |
| 41  | DG    | 81  | LYS  |
| 41  | DG    | 82  | LEU  |
| 41  | DG    | 87  | PRO  |
| 41  | DG    | 96  | ARG  |
| 41  | DG    | 109 | VAL  |
| 41  | DG    | 110 | ALA  |
| 42  | DH    | 13  | LYS  |
| 42  | DH    | 20  | ALA  |
| 42  | DH    | 41  | MET  |
| 42  | DH    | 46  | GLU  |
| 42  | DH    | 55  | PRO  |
| 42  | DH    | 83  | TYR  |
| 42  | DH    | 154 | PRO  |
| 42  | DH    | 155 | SER  |
| 42  | DH    | 156 | ALA  |
| 42  | DH    | 157 | TYR  |
| 42  | DH    | 160 | LYS  |
| 42  | DH    | 169 | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | DH    | 173 | PRO  |
| 42  | DH    | 176 | ALA  |
| 44  | DK    | 51  | ALA  |
| 44  | DK    | 115 | LEU  |
| 46  | DN    | 8   | GLN  |
| 46  | DN    | 36  | GLY  |
| 46  | DN    | 46  | VAL  |
| 46  | DN    | 47  | ALA  |
| 46  | DN    | 58  | ASP  |
| 46  | DN    | 63  | THR  |
| 46  | DN    | 130 | HIS  |
| 46  | DN    | 133 | GLN  |
| 47  | DO    | 35  | VAL  |
| 47  | DO    | 48  | PRO  |
| 47  | DO    | 68  | GLU  |
| 48  | DP    | 12  | ALA  |
| 48  | DP    | 14  | LYS  |
| 48  | DP    | 17  | LYS  |
| 48  | DP    | 31  | ALA  |
| 48  | DP    | 47  | ASP  |
| 48  | DP    | 48  | PRO  |
| 48  | DP    | 52  | GLU  |
| 48  | DP    | 57  | THR  |
| 48  | DP    | 58  | THR  |
| 48  | DP    | 111 | ARG  |
| 48  | DP    | 135 | LEU  |
| 48  | DP    | 147 | LEU  |
| 49  | DQ    | 27  | VAL  |
| 49  | DQ    | 135 | ASP  |
| 50  | DR    | 8   | ARG  |
| 50  | DR    | 14  | SER  |
| 50  | DR    | 58  | GLY  |
| 50  | DR    | 88  | ARG  |
| 50  | DR    | 107 | ASP  |
| 50  | DR    | 117 | VAL  |
| 51  | DS    | 13  | ARG  |
| 51  | DS    | 23  | ARG  |
| 51  | DS    | 57  | LYS  |
| 51  | DS    | 97  | ARG  |
| 51  | DS    | 100 | ALA  |
| 51  | DS    | 102 | ALA  |
| 51  | DS    | 103 | GLU  |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 52         | DT           | 5          | ALA         |
| 52         | DT           | 6          | LEU         |
| 52         | DT           | 24         | PRO         |
| 52         | DT           | 28         | VAL         |
| 52         | DT           | 30         | VAL         |
| 52         | DT           | 55         | ASN         |
| 52         | DT           | 80         | SER         |
| 52         | DT           | 91         | ARG         |
| 52         | DT           | 97         | ALA         |
| 52         | DT           | 104        | ASN         |
| 52         | DT           | 107        | ASP         |
| 52         | DT           | 130        | ALA         |
| 52         | DT           | 132        | LYS         |
| 52         | DT           | 135        | ALA         |
| 53         | DU           | 91         | ASP         |
| 53         | DU           | 93         | LYS         |
| 54         | DV           | 16         | PRO         |
| 54         | DV           | 18         | LEU         |
| 54         | DV           | 19         | LYS         |
| 54         | DV           | 46         | VAL         |
| 54         | DV           | 67         | GLY         |
| 55         | DW           | 63         | ASP         |
| 56         | DX           | 12         | VAL         |
| 56         | DX           | 42         | ALA         |
| 57         | DY           | 7          | VAL         |
| 57         | DY           | 24         | VAL         |
| 57         | DY           | 48         | ALA         |
| 57         | DY           | 60         | PHE         |
| 57         | DY           | 74         | PRO         |
| 57         | DY           | 77         | PRO         |
| 57         | DY           | 78         | ALA         |
| 57         | DY           | 99         | CYS         |
| 57         | DY           | 100        | ALA         |
| 57         | DY           | 104        | GLY         |
| 58         | DZ           | 38         | TYR         |
| 58         | DZ           | 42         | VAL         |
| 58         | DZ           | 80         | ARG         |
| 58         | DZ           | 112        | ARG         |
| 58         | DZ           | 136        | PHE         |
| 58         | DZ           | 146        | ILE         |
| 58         | DZ           | 158        | PRO         |
| 58         | DZ           | 177        | PRO         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 58  | DZ    | 181 | GLU  |
| 58  | DZ    | 186 | GLU  |
| 2   | AB    | 18  | GLY  |
| 2   | AB    | 24  | TRP  |
| 2   | AB    | 65  | GLY  |
| 2   | AB    | 83  | MET  |
| 2   | AB    | 128 | GLU  |
| 2   | AB    | 151 | GLY  |
| 2   | AB    | 152 | PHE  |
| 2   | AB    | 153 | ARG  |
| 2   | AB    | 165 | VAL  |
| 2   | AB    | 216 | SER  |
| 2   | AB    | 221 | LEU  |
| 2   | AB    | 224 | GLN  |
| 2   | AB    | 238 | LEU  |
| 3   | AC    | 26  | LYS  |
| 3   | AC    | 96  | GLY  |
| 3   | AC    | 129 | ALA  |
| 3   | AC    | 131 | ARG  |
| 3   | AC    | 135 | LYS  |
| 3   | AC    | 139 | GLN  |
| 4   | AD    | 5   | ILE  |
| 4   | AD    | 69  | GLY  |
| 4   | AD    | 156 | GLU  |
| 4   | AD    | 171 | GLY  |
| 5   | AE    | 8   | GLU  |
| 6   | AF    | 30  | LEU  |
| 6   | AF    | 34  | GLY  |
| 6   | AF    | 43  | LEU  |
| 7   | AG    | 80  | VAL  |
| 8   | AH    | 2   | LEU  |
| 9   | AI    | 34  | ASN  |
| 9   | AI    | 85  | LEU  |
| 10  | AJ    | 19  | SER  |
| 10  | AJ    | 61  | GLU  |
| 10  | AJ    | 83  | GLU  |
| 10  | AJ    | 84  | GLN  |
| 10  | AJ    | 85  | LEU  |
| 11  | AK    | 88  | GLY  |
| 12  | AL    | 46  | LYS  |
| 12  | AL    | 71  | PRO  |
| 12  | AL    | 87  | GLY  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | AL    | 89  | ARG  |
| 12  | AL    | 121 | GLY  |
| 13  | AM    | 4   | ILE  |
| 13  | AM    | 5   | ALA  |
| 13  | AM    | 7   | VAL  |
| 13  | AM    | 55  | ARG  |
| 13  | AM    | 114 | ARG  |
| 14  | AN    | 14  | PRO  |
| 16  | AP    | 34  | GLU  |
| 18  | AR    | 41  | LYS  |
| 19  | AS    | 14  | HIS  |
| 19  | AS    | 25  | LYS  |
| 19  | AS    | 26  | GLY  |
| 19  | AS    | 62  | ILE  |
| 19  | AS    | 63  | THR  |
| 19  | AS    | 73  | GLU  |
| 20  | AT    | 49  | ALA  |
| 20  | AT    | 62  | LEU  |
| 20  | AT    | 69  | GLY  |
| 24  | AY    | 10  | LYS  |
| 24  | AY    | 39  | ILE  |
| 24  | AY    | 112 | GLN  |
| 24  | AY    | 114 | VAL  |
| 24  | AY    | 183 | MET  |
| 24  | AY    | 196 | ILE  |
| 24  | AY    | 299 | VAL  |
| 24  | AY    | 347 | GLY  |
| 24  | AY    | 371 | ALA  |
| 24  | AY    | 380 | LEU  |
| 24  | AY    | 386 | GLY  |
| 24  | AY    | 399 | LEU  |
| 24  | AY    | 416 | LYS  |
| 24  | AY    | 418 | LYS  |
| 24  | AY    | 471 | LYS  |
| 24  | AY    | 505 | GLY  |
| 24  | AY    | 657 | THR  |
| 24  | AY    | 678 | GLU  |
| 25  | B0    | 20  | ARG  |
| 26  | B1    | 69  | LYS  |
| 26  | B1    | 84  | GLY  |
| 27  | B2    | 21  | LEU  |
| 27  | B2    | 26  | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | B2    | 49  | LYS  |
| 28  | B3    | 29  | ARG  |
| 29  | B4    | 5   | ILE  |
| 29  | B4    | 9   | LEU  |
| 29  | B4    | 20  | ASN  |
| 29  | B4    | 44  | THR  |
| 29  | B4    | 48  | ARG  |
| 29  | B4    | 51  | ASP  |
| 30  | B5    | 35  | GLU  |
| 30  | B5    | 36  | CYS  |
| 30  | B5    | 38  | ALA  |
| 30  | B5    | 58  | LEU  |
| 30  | B5    | 59  | GLU  |
| 31  | B6    | 16  | CYS  |
| 31  | B6    | 19  | ARG  |
| 31  | B6    | 23  | THR  |
| 31  | B6    | 28  | ARG  |
| 31  | B6    | 43  | CYS  |
| 32  | B7    | 17  | GLY  |
| 33  | B8    | 34  | TRP  |
| 33  | B8    | 37  | SER  |
| 33  | B8    | 40  | GLU  |
| 34  | B9    | 11  | CYS  |
| 34  | B9    | 12  | ASP  |
| 37  | BC    | 12  | LEU  |
| 37  | BC    | 30  | VAL  |
| 37  | BC    | 38  | PHE  |
| 38  | BD    | 3   | VAL  |
| 38  | BD    | 12  | SER  |
| 38  | BD    | 32  | SER  |
| 38  | BD    | 36  | PRO  |
| 38  | BD    | 42  | GLY  |
| 38  | BD    | 125 | ILE  |
| 38  | BD    | 197 | GLY  |
| 38  | BD    | 198 | ASN  |
| 38  | BD    | 234 | GLY  |
| 38  | BD    | 260 | ARG  |
| 38  | BD    | 267 | SER  |
| 38  | BD    | 268 | ARG  |
| 39  | BE    | 2   | LYS  |
| 39  | BE    | 46  | ALA  |
| 39  | BE    | 53  | PRO  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | BE    | 57  | LYS  |
| 39  | BE    | 66  | HIS  |
| 39  | BE    | 69  | LYS  |
| 39  | BE    | 71  | GLY  |
| 39  | BE    | 72  | VAL  |
| 39  | BE    | 118 | LYS  |
| 39  | BE    | 134 | ILE  |
| 39  | BE    | 144 | ARG  |
| 39  | BE    | 186 | GLY  |
| 40  | BF    | 5   | ALA  |
| 40  | BF    | 10  | PRO  |
| 40  | BF    | 84  | VAL  |
| 40  | BF    | 127 | GLU  |
| 40  | BF    | 169 | ASN  |
| 40  | BF    | 181 | LEU  |
| 40  | BF    | 206 | ILE  |
| 40  | BF    | 207 | GLY  |
| 41  | BG    | 14  | GLU  |
| 41  | BG    | 75  | LYS  |
| 41  | BG    | 81  | LYS  |
| 41  | BG    | 82  | LEU  |
| 41  | BG    | 166 | ASP  |
| 42  | BH    | 21  | PRO  |
| 42  | BH    | 42  | ARG  |
| 42  | BH    | 69  | ARG  |
| 42  | BH    | 138 | LYS  |
| 42  | BH    | 174 | GLY  |
| 42  | BH    | 176 | ALA  |
| 44  | BK    | 10  | LEU  |
| 44  | BK    | 42  | ASN  |
| 44  | BK    | 48  | MET  |
| 44  | BK    | 62  | ASP  |
| 44  | BK    | 82  | ALA  |
| 44  | BK    | 87  | GLY  |
| 46  | BN    | 77  | GLY  |
| 46  | BN    | 125 | GLY  |
| 46  | BN    | 129 | PRO  |
| 47  | BO    | 5   | GLN  |
| 47  | BO    | 29  | ASN  |
| 47  | BO    | 89  | ASN  |
| 47  | BO    | 100 | GLY  |
| 48  | BP    | 34  | GLY  |

*Continued on next page...*



*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 48         | BP           | 98         | GLU         |
| 49         | BQ           | 52         | VAL         |
| 49         | BQ           | 62         | GLY         |
| 49         | BQ           | 71         | ASP         |
| 50         | BR           | 45         | ARG         |
| 50         | BR           | 83         | ILE         |
| 51         | BS           | 37         | ALA         |
| 51         | BS           | 57         | LYS         |
| 51         | BS           | 59         | LYS         |
| 51         | BS           | 85         | VAL         |
| 51         | BS           | 94         | TYR         |
| 51         | BS           | 104        | GLY         |
| 51         | BS           | 107        | GLU         |
| 52         | BT           | 11         | GLU         |
| 52         | BT           | 12         | SER         |
| 52         | BT           | 58         | ASN         |
| 52         | BT           | 88         | ILE         |
| 52         | BT           | 97         | ALA         |
| 52         | BT           | 133        | GLU         |
| 53         | BU           | 11         | ARG         |
| 53         | BU           | 27         | LEU         |
| 53         | BU           | 32         | PHE         |
| 53         | BU           | 67         | ALA         |
| 54         | BV           | 2          | PHE         |
| 54         | BV           | 26         | ASP         |
| 54         | BV           | 31         | ALA         |
| 54         | BV           | 47         | VAL         |
| 54         | BV           | 53         | GLU         |
| 54         | BV           | 55         | ALA         |
| 54         | BV           | 78         | LYS         |
| 55         | BW           | 6          | ILE         |
| 55         | BW           | 11         | ARG         |
| 56         | BX           | 87         | GLN         |
| 57         | BY           | 17         | SER         |
| 57         | BY           | 38         | ILE         |
| 57         | BY           | 39         | VAL         |
| 57         | BY           | 41         | GLY         |
| 57         | BY           | 59         | GLY         |
| 57         | BY           | 81         | LYS         |
| 57         | BY           | 98         | VAL         |
| 57         | BY           | 107        | ASP         |
| 58         | BZ           | 5          | LEU         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 58  | BZ    | 42  | VAL  |
| 58  | BZ    | 85  | HIS  |
| 58  | BZ    | 112 | ARG  |
| 58  | BZ    | 148 | ASP  |
| 58  | BZ    | 158 | PRO  |
| 58  | BZ    | 180 | VAL  |
| 2   | CB    | 18  | GLY  |
| 2   | CB    | 24  | TRP  |
| 2   | CB    | 65  | GLY  |
| 2   | CB    | 83  | MET  |
| 2   | CB    | 128 | GLU  |
| 2   | CB    | 151 | GLY  |
| 2   | CB    | 152 | PHE  |
| 2   | CB    | 153 | ARG  |
| 2   | CB    | 165 | VAL  |
| 2   | CB    | 190 | THR  |
| 2   | CB    | 216 | SER  |
| 2   | CB    | 221 | LEU  |
| 2   | CB    | 224 | GLN  |
| 2   | CB    | 236 | TYR  |
| 2   | CB    | 238 | LEU  |
| 3   | CC    | 26  | LYS  |
| 3   | CC    | 96  | GLY  |
| 3   | CC    | 129 | ALA  |
| 3   | CC    | 131 | ARG  |
| 3   | CC    | 135 | LYS  |
| 3   | CC    | 139 | GLN  |
| 4   | CD    | 5   | ILE  |
| 4   | CD    | 31  | CYS  |
| 4   | CD    | 69  | GLY  |
| 4   | CD    | 156 | GLU  |
| 4   | CD    | 179 | GLU  |
| 5   | CE    | 8   | GLU  |
| 6   | CF    | 30  | LEU  |
| 6   | CF    | 34  | GLY  |
| 6   | CF    | 43  | LEU  |
| 7   | CG    | 41  | ARG  |
| 7   | CG    | 80  | VAL  |
| 8   | CH    | 2   | LEU  |
| 9   | CI    | 34  | ASN  |
| 10  | CJ    | 19  | SER  |
| 10  | CJ    | 61  | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | CJ    | 84  | GLN  |
| 10  | CJ    | 85  | LEU  |
| 11  | CK    | 88  | GLY  |
| 12  | CL    | 46  | LYS  |
| 12  | CL    | 71  | PRO  |
| 12  | CL    | 72  | GLY  |
| 12  | CL    | 87  | GLY  |
| 12  | CL    | 89  | ARG  |
| 12  | CL    | 121 | GLY  |
| 13  | CM    | 4   | ILE  |
| 13  | CM    | 5   | ALA  |
| 13  | CM    | 7   | VAL  |
| 13  | CM    | 55  | ARG  |
| 13  | CM    | 114 | ARG  |
| 13  | CM    | 121 | LYS  |
| 16  | CP    | 34  | GLU  |
| 16  | CP    | 76  | GLN  |
| 17  | CQ    | 95  | TYR  |
| 18  | CR    | 41  | LYS  |
| 19  | CS    | 14  | HIS  |
| 19  | CS    | 25  | LYS  |
| 19  | CS    | 26  | GLY  |
| 19  | CS    | 62  | ILE  |
| 19  | CS    | 63  | THR  |
| 19  | CS    | 73  | GLU  |
| 20  | CT    | 49  | ALA  |
| 20  | CT    | 62  | LEU  |
| 20  | CT    | 69  | GLY  |
| 24  | CY    | 34  | TYR  |
| 24  | CY    | 86  | GLY  |
| 24  | CY    | 112 | GLN  |
| 24  | CY    | 127 | LYS  |
| 24  | CY    | 129 | LYS  |
| 24  | CY    | 143 | GLY  |
| 24  | CY    | 144 | ALA  |
| 24  | CY    | 172 | ASP  |
| 24  | CY    | 203 | GLU  |
| 24  | CY    | 211 | GLU  |
| 24  | CY    | 300 | GLU  |
| 24  | CY    | 366 | VAL  |
| 24  | CY    | 416 | LYS  |
| 24  | CY    | 505 | GLY  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | CY    | 531 | GLY  |
| 24  | CY    | 537 | GLU  |
| 24  | CY    | 547 | GLU  |
| 24  | CY    | 551 | GLN  |
| 24  | CY    | 595 | GLN  |
| 24  | CY    | 664 | GLN  |
| 24  | CY    | 673 | PHE  |
| 24  | CY    | 681 | LYS  |
| 25  | D0    | 20  | ARG  |
| 26  | D1    | 22  | GLY  |
| 26  | D1    | 30  | VAL  |
| 26  | D1    | 83  | GLU  |
| 26  | D1    | 84  | GLY  |
| 26  | D1    | 85  | LEU  |
| 26  | D1    | 94  | LEU  |
| 26  | D1    | 95  | LEU  |
| 27  | D2    | 5   | GLU  |
| 27  | D2    | 49  | LYS  |
| 28  | D3    | 29  | ARG  |
| 29  | D4    | 3   | GLU  |
| 29  | D4    | 5   | ILE  |
| 29  | D4    | 9   | LEU  |
| 29  | D4    | 20  | ASN  |
| 29  | D4    | 44  | THR  |
| 29  | D4    | 48  | ARG  |
| 29  | D4    | 51  | ASP  |
| 30  | D5    | 35  | GLU  |
| 30  | D5    | 36  | CYS  |
| 30  | D5    | 38  | ALA  |
| 30  | D5    | 58  | LEU  |
| 30  | D5    | 59  | GLU  |
| 31  | D6    | 16  | CYS  |
| 31  | D6    | 19  | ARG  |
| 31  | D6    | 23  | THR  |
| 31  | D6    | 28  | ARG  |
| 32  | D7    | 17  | GLY  |
| 33  | D8    | 34  | TRP  |
| 33  | D8    | 37  | SER  |
| 33  | D8    | 40  | GLU  |
| 34  | D9    | 11  | CYS  |
| 34  | D9    | 12  | ASP  |
| 37  | DC    | 12  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | DC    | 30  | VAL  |
| 37  | DC    | 38  | PHE  |
| 38  | DD    | 3   | VAL  |
| 38  | DD    | 12  | SER  |
| 38  | DD    | 30  | GLU  |
| 38  | DD    | 32  | SER  |
| 38  | DD    | 36  | PRO  |
| 38  | DD    | 41  | GLY  |
| 38  | DD    | 42  | GLY  |
| 38  | DD    | 125 | ILE  |
| 38  | DD    | 197 | GLY  |
| 38  | DD    | 198 | ASN  |
| 38  | DD    | 236 | GLY  |
| 38  | DD    | 267 | SER  |
| 38  | DD    | 268 | ARG  |
| 39  | DE    | 2   | LYS  |
| 39  | DE    | 46  | ALA  |
| 39  | DE    | 53  | PRO  |
| 39  | DE    | 57  | LYS  |
| 39  | DE    | 66  | HIS  |
| 39  | DE    | 69  | LYS  |
| 39  | DE    | 71  | GLY  |
| 39  | DE    | 72  | VAL  |
| 39  | DE    | 118 | LYS  |
| 39  | DE    | 129 | HIS  |
| 39  | DE    | 134 | ILE  |
| 39  | DE    | 144 | ARG  |
| 39  | DE    | 186 | GLY  |
| 40  | DF    | 10  | PRO  |
| 40  | DF    | 82  | ILE  |
| 40  | DF    | 84  | VAL  |
| 40  | DF    | 127 | GLU  |
| 40  | DF    | 169 | ASN  |
| 40  | DF    | 181 | LEU  |
| 40  | DF    | 206 | ILE  |
| 41  | DG    | 3   | LEU  |
| 41  | DG    | 76  | SER  |
| 41  | DG    | 104 | GLU  |
| 41  | DG    | 124 | SER  |
| 41  | DG    | 181 | ARG  |
| 42  | DH    | 21  | PRO  |
| 42  | DH    | 42  | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | DH    | 69  | ARG  |
| 42  | DH    | 138 | LYS  |
| 44  | DK    | 10  | LEU  |
| 44  | DK    | 42  | ASN  |
| 44  | DK    | 48  | MET  |
| 44  | DK    | 62  | ASP  |
| 44  | DK    | 82  | ALA  |
| 44  | DK    | 87  | GLY  |
| 46  | DN    | 57  | ALA  |
| 46  | DN    | 77  | GLY  |
| 46  | DN    | 125 | GLY  |
| 46  | DN    | 129 | PRO  |
| 47  | DO    | 5   | GLN  |
| 47  | DO    | 29  | ASN  |
| 47  | DO    | 54  | GLU  |
| 47  | DO    | 89  | ASN  |
| 47  | DO    | 120 | GLU  |
| 48  | DP    | 34  | GLY  |
| 48  | DP    | 98  | GLU  |
| 49  | DQ    | 52  | VAL  |
| 49  | DQ    | 62  | GLY  |
| 49  | DQ    | 71  | ASP  |
| 50  | DR    | 45  | ARG  |
| 51  | DS    | 37  | ALA  |
| 51  | DS    | 59  | LYS  |
| 51  | DS    | 85  | VAL  |
| 51  | DS    | 94  | TYR  |
| 51  | DS    | 104 | GLY  |
| 51  | DS    | 107 | GLU  |
| 52  | DT    | 12  | SER  |
| 52  | DT    | 41  | ARG  |
| 52  | DT    | 88  | ILE  |
| 52  | DT    | 133 | GLU  |
| 53  | DU    | 11  | ARG  |
| 53  | DU    | 27  | LEU  |
| 53  | DU    | 32  | PHE  |
| 53  | DU    | 67  | ALA  |
| 54  | DV    | 2   | PHE  |
| 54  | DV    | 26  | ASP  |
| 54  | DV    | 31  | ALA  |
| 54  | DV    | 47  | VAL  |
| 54  | DV    | 53  | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | DV    | 55  | ALA  |
| 55  | DW    | 6   | ILE  |
| 55  | DW    | 11  | ARG  |
| 56  | DX    | 87  | GLN  |
| 57  | DY    | 17  | SER  |
| 57  | DY    | 38  | ILE  |
| 57  | DY    | 39  | VAL  |
| 57  | DY    | 41  | GLY  |
| 57  | DY    | 59  | GLY  |
| 57  | DY    | 81  | LYS  |
| 57  | DY    | 92  | ASN  |
| 57  | DY    | 98  | VAL  |
| 57  | DY    | 107 | ASP  |
| 58  | DZ    | 17  | ALA  |
| 58  | DZ    | 18  | LEU  |
| 58  | DZ    | 37  | VAL  |
| 58  | DZ    | 40  | ASP  |
| 58  | DZ    | 142 | SER  |
| 58  | DZ    | 148 | ASP  |
| 58  | DZ    | 159 | PRO  |
| 2   | AB    | 78  | GLN  |
| 2   | AB    | 79  | ASP  |
| 2   | AB    | 236 | TYR  |
| 3   | AC    | 4   | LYS  |
| 3   | AC    | 168 | ALA  |
| 4   | AD    | 31  | CYS  |
| 4   | AD    | 40  | PRO  |
| 5   | AE    | 140 | ARG  |
| 5   | AE    | 154 | GLY  |
| 7   | AG    | 14  | PRO  |
| 7   | AG    | 41  | ARG  |
| 7   | AG    | 62  | PHE  |
| 9   | AI    | 11  | LYS  |
| 9   | AI    | 44  | VAL  |
| 9   | AI    | 95  | LYS  |
| 12  | AL    | 47  | LYS  |
| 12  | AL    | 51  | ALA  |
| 12  | AL    | 72  | GLY  |
| 12  | AL    | 92  | ASP  |
| 13  | AM    | 11  | ARG  |
| 13  | AM    | 121 | LYS  |
| 14  | AN    | 16  | PHE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | AO    | 14  | GLU  |
| 15  | AO    | 77  | ARG  |
| 16  | AP    | 13  | HIS  |
| 16  | AP    | 76  | GLN  |
| 17  | AQ    | 95  | TYR  |
| 20  | AT    | 97  | ALA  |
| 24  | AY    | 25  | LYS  |
| 24  | AY    | 34  | TYR  |
| 24  | AY    | 42  | ILE  |
| 24  | AY    | 89  | ASP  |
| 24  | AY    | 120 | THR  |
| 24  | AY    | 144 | ALA  |
| 24  | AY    | 148 | LEU  |
| 24  | AY    | 283 | PRO  |
| 24  | AY    | 393 | ASP  |
| 24  | AY    | 458 | HIS  |
| 24  | AY    | 469 | GLU  |
| 24  | AY    | 532 | GLY  |
| 24  | AY    | 535 | PRO  |
| 24  | AY    | 636 | PRO  |
| 24  | AY    | 680 | PRO  |
| 26  | B1    | 95  | LEU  |
| 27  | B2    | 43  | GLN  |
| 27  | B2    | 58  | ALA  |
| 27  | B2    | 68  | ARG  |
| 28  | B3    | 32  | GLN  |
| 30  | B5    | 37  | LYS  |
| 33  | B8    | 35  | GLN  |
| 33  | B8    | 57  | ARG  |
| 37  | BC    | 17  | PRO  |
| 37  | BC    | 127 | LYS  |
| 38  | BD    | 28  | GLU  |
| 38  | BD    | 41  | GLY  |
| 38  | BD    | 74  | GLY  |
| 38  | BD    | 129 | ASN  |
| 38  | BD    | 134 | ARG  |
| 38  | BD    | 236 | GLY  |
| 38  | BD    | 242 | ARG  |
| 39  | BE    | 83  | ASP  |
| 39  | BE    | 86  | PRO  |
| 39  | BE    | 117 | MET  |
| 39  | BE    | 129 | HIS  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | BF    | 3   | GLU  |
| 40  | BF    | 82  | ILE  |
| 40  | BF    | 108 | LYS  |
| 40  | BF    | 115 | ALA  |
| 40  | BF    | 122 | LYS  |
| 40  | BF    | 168 | ARG  |
| 40  | BF    | 195 | ASP  |
| 41  | BG    | 22  | ARG  |
| 41  | BG    | 43  | LEU  |
| 41  | BG    | 116 | ASP  |
| 41  | BG    | 163 | ALA  |
| 42  | BH    | 18  | GLU  |
| 42  | BH    | 47  | GLU  |
| 42  | BH    | 85  | LYS  |
| 42  | BH    | 98  | LEU  |
| 42  | BH    | 126 | PRO  |
| 42  | BH    | 158 | HIS  |
| 42  | BH    | 165 | ALA  |
| 42  | BH    | 170 | ARG  |
| 42  | BH    | 171 | LEU  |
| 46  | BN    | 40  | PRO  |
| 46  | BN    | 59  | LYS  |
| 46  | BN    | 110 | GLY  |
| 46  | BN    | 136 | GLU  |
| 47  | BO    | 120 | GLU  |
| 48  | BP    | 43  | GLY  |
| 48  | BP    | 49  | ARG  |
| 48  | BP    | 123 | LEU  |
| 50  | BR    | 12  | ARG  |
| 51  | BS    | 71  | ARG  |
| 51  | BS    | 90  | GLY  |
| 51  | BS    | 99  | LYS  |
| 52  | BT    | 3   | ARG  |
| 52  | BT    | 41  | ARG  |
| 52  | BT    | 103 | ARG  |
| 53  | BU    | 83  | LEU  |
| 53  | BU    | 114 | LYS  |
| 54  | BV    | 3   | ALA  |
| 54  | BV    | 50  | PRO  |
| 55  | BW    | 18  | ARG  |
| 56  | BX    | 19  | ALA  |
| 56  | BX    | 22  | ALA  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 56  | BX    | 91  | ALA  |
| 57  | BY    | 46  | LYS  |
| 57  | BY    | 92  | ASN  |
| 58  | BZ    | 30  | ASN  |
| 58  | BZ    | 83  | PRO  |
| 58  | BZ    | 122 | ARG  |
| 58  | BZ    | 128 | VAL  |
| 58  | BZ    | 166 | SER  |
| 58  | BZ    | 170 | THR  |
| 2   | CB    | 78  | GLN  |
| 2   | CB    | 79  | ASP  |
| 3   | CC    | 4   | LYS  |
| 3   | CC    | 15  | THR  |
| 3   | CC    | 168 | ALA  |
| 4   | CD    | 40  | PRO  |
| 5   | CE    | 154 | GLY  |
| 6   | CF    | 29  | ALA  |
| 7   | CG    | 14  | PRO  |
| 7   | CG    | 62  | PHE  |
| 9   | CI    | 11  | LYS  |
| 9   | CI    | 44  | VAL  |
| 9   | CI    | 85  | LEU  |
| 9   | CI    | 95  | LYS  |
| 10  | CJ    | 83  | GLU  |
| 12  | CL    | 47  | LYS  |
| 12  | CL    | 51  | ALA  |
| 12  | CL    | 92  | ASP  |
| 12  | CL    | 116 | SER  |
| 13  | CM    | 11  | ARG  |
| 14  | CN    | 14  | PRO  |
| 14  | CN    | 16  | PHE  |
| 15  | CO    | 14  | GLU  |
| 15  | CO    | 77  | ARG  |
| 16  | CP    | 13  | HIS  |
| 19  | CS    | 5   | LEU  |
| 20  | CT    | 97  | ALA  |
| 24  | CY    | 87  | HIS  |
| 24  | CY    | 91  | THR  |
| 24  | CY    | 123 | ARG  |
| 24  | CY    | 192 | LEU  |
| 24  | CY    | 239 | GLU  |
| 24  | CY    | 303 | PRO  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | CY    | 380 | LEU  |
| 24  | CY    | 400 | GLU  |
| 24  | CY    | 421 | GLN  |
| 24  | CY    | 458 | HIS  |
| 24  | CY    | 502 | GLY  |
| 24  | CY    | 504 | ARG  |
| 24  | CY    | 519 | ARG  |
| 24  | CY    | 620 | VAL  |
| 24  | CY    | 680 | PRO  |
| 27  | D2    | 4   | SER  |
| 27  | D2    | 41  | ILE  |
| 27  | D2    | 68  | ARG  |
| 27  | D2    | 71  | ASN  |
| 28  | D3    | 32  | GLN  |
| 30  | D5    | 37  | LYS  |
| 31  | D6    | 43  | CYS  |
| 33  | D8    | 35  | GLN  |
| 33  | D8    | 57  | ARG  |
| 37  | DC    | 17  | PRO  |
| 37  | DC    | 82  | GLU  |
| 37  | DC    | 127 | LYS  |
| 38  | DD    | 28  | GLU  |
| 38  | DD    | 74  | GLY  |
| 38  | DD    | 129 | ASN  |
| 38  | DD    | 134 | ARG  |
| 38  | DD    | 234 | GLY  |
| 38  | DD    | 242 | ARG  |
| 38  | DD    | 260 | ARG  |
| 39  | DE    | 83  | ASP  |
| 39  | DE    | 86  | PRO  |
| 40  | DF    | 3   | GLU  |
| 40  | DF    | 5   | ALA  |
| 40  | DF    | 108 | LYS  |
| 40  | DF    | 115 | ALA  |
| 40  | DF    | 126 | VAL  |
| 40  | DF    | 168 | ARG  |
| 40  | DF    | 195 | ASP  |
| 40  | DF    | 207 | GLY  |
| 41  | DG    | 21  | ARG  |
| 41  | DG    | 115 | ARG  |
| 41  | DG    | 117 | PHE  |
| 41  | DG    | 169 | ALA  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | DH    | 18  | GLU  |
| 42  | DH    | 47  | GLU  |
| 42  | DH    | 85  | LYS  |
| 42  | DH    | 98  | LEU  |
| 42  | DH    | 126 | PRO  |
| 42  | DH    | 158 | HIS  |
| 42  | DH    | 165 | ALA  |
| 42  | DH    | 170 | ARG  |
| 42  | DH    | 171 | LEU  |
| 42  | DH    | 174 | GLY  |
| 46  | DN    | 40  | PRO  |
| 46  | DN    | 59  | LYS  |
| 46  | DN    | 110 | GLY  |
| 46  | DN    | 136 | GLU  |
| 47  | DO    | 100 | GLY  |
| 48  | DP    | 43  | GLY  |
| 48  | DP    | 49  | ARG  |
| 48  | DP    | 123 | LEU  |
| 50  | DR    | 12  | ARG  |
| 50  | DR    | 83  | ILE  |
| 51  | DS    | 71  | ARG  |
| 51  | DS    | 90  | GLY  |
| 51  | DS    | 99  | LYS  |
| 52  | DT    | 11  | GLU  |
| 52  | DT    | 58  | ASN  |
| 53  | DU    | 66  | ASN  |
| 53  | DU    | 83  | LEU  |
| 53  | DU    | 110 | VAL  |
| 53  | DU    | 114 | LYS  |
| 54  | DV    | 3   | ALA  |
| 54  | DV    | 50  | PRO  |
| 54  | DV    | 78  | LYS  |
| 55  | DW    | 18  | ARG  |
| 56  | DX    | 6   | ASP  |
| 56  | DX    | 19  | ALA  |
| 56  | DX    | 22  | ALA  |
| 56  | DX    | 91  | ALA  |
| 57  | DY    | 46  | LYS  |
| 57  | DY    | 75  | ILE  |
| 58  | DZ    | 49  | ARG  |
| 58  | DZ    | 81  | ARG  |
| 58  | DZ    | 108 | PRO  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 58  | DZ    | 168 | GLU  |
| 2   | AB    | 29  | ALA  |
| 2   | AB    | 63  | MET  |
| 2   | AB    | 64  | ARG  |
| 2   | AB    | 97  | TRP  |
| 2   | AB    | 130 | ARG  |
| 3   | AC    | 15  | THR  |
| 3   | AC    | 44  | GLU  |
| 3   | AC    | 63  | ASN  |
| 3   | AC    | 65  | ALA  |
| 4   | AD    | 71  | SER  |
| 5   | AE    | 37  | ARG  |
| 5   | AE    | 136 | MET  |
| 5   | AE    | 138 | ALA  |
| 6   | AF    | 29  | ALA  |
| 10  | AJ    | 23  | ILE  |
| 10  | AJ    | 32  | ALA  |
| 12  | AL    | 19  | ARG  |
| 12  | AL    | 116 | SER  |
| 13  | AM    | 36  | LYS  |
| 13  | AM    | 113 | PRO  |
| 15  | AO    | 26  | GLU  |
| 15  | AO    | 80  | ALA  |
| 15  | AO    | 84  | LYS  |
| 17  | AQ    | 89  | LEU  |
| 19  | AS    | 5   | LEU  |
| 19  | AS    | 42  | PRO  |
| 19  | AS    | 50  | ALA  |
| 20  | AT    | 85  | MET  |
| 20  | AT    | 96  | GLY  |
| 20  | AT    | 98  | PRO  |
| 21  | AU    | 25  | LYS  |
| 24  | AY    | 230 | LYS  |
| 24  | AY    | 406 | GLU  |
| 24  | AY    | 444 | PRO  |
| 24  | AY    | 457 | LEU  |
| 24  | AY    | 502 | GLY  |
| 24  | AY    | 506 | GLN  |
| 24  | AY    | 549 | ALA  |
| 26  | B1    | 54  | ALA  |
| 27  | B2    | 51  | ARG  |
| 27  | B2    | 70  | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | B6    | 41  | PRO  |
| 33  | B8    | 3   | LYS  |
| 34  | B9    | 30  | PRO  |
| 37  | BC    | 82  | GLU  |
| 37  | BC    | 168 | LYS  |
| 37  | BC    | 227 | PRO  |
| 39  | BE    | 17  | ASP  |
| 39  | BE    | 64  | LYS  |
| 39  | BE    | 70  | ALA  |
| 39  | BE    | 82  | ARG  |
| 40  | BF    | 62  | ARG  |
| 40  | BF    | 126 | VAL  |
| 40  | BF    | 134 | GLY  |
| 40  | BF    | 180 | GLY  |
| 41  | BG    | 30  | GLU  |
| 41  | BG    | 103 | LEU  |
| 41  | BG    | 126 | ASP  |
| 44  | BK    | 116 | ASN  |
| 48  | BP    | 89  | ALA  |
| 48  | BP    | 106 | LEU  |
| 48  | BP    | 107 | LYS  |
| 48  | BP    | 108 | LYS  |
| 48  | BP    | 119 | GLU  |
| 49  | BQ    | 139 | GLU  |
| 50  | BR    | 31  | HIS  |
| 50  | BR    | 61  | HIS  |
| 50  | BR    | 86  | ARG  |
| 51  | BS    | 15  | ARG  |
| 51  | BS    | 89  | ARG  |
| 51  | BS    | 105 | ALA  |
| 52  | BT    | 26  | ASP  |
| 53  | BU    | 66  | ASN  |
| 53  | BU    | 110 | VAL  |
| 55  | BW    | 111 | HIS  |
| 56  | BX    | 6   | ASP  |
| 57  | BY    | 67  | LEU  |
| 57  | BY    | 75  | ILE  |
| 58  | BZ    | 71  | VAL  |
| 58  | BZ    | 159 | PRO  |
| 58  | BZ    | 165 | VAL  |
| 2   | CB    | 29  | ALA  |
| 2   | CB    | 63  | MET  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | CB    | 64  | ARG  |
| 2   | CB    | 97  | TRP  |
| 2   | CB    | 130 | ARG  |
| 2   | CB    | 212 | GLN  |
| 3   | CC    | 65  | ALA  |
| 4   | CD    | 149 | ALA  |
| 5   | CE    | 37  | ARG  |
| 5   | CE    | 136 | MET  |
| 5   | CE    | 138 | ALA  |
| 5   | CE    | 140 | ARG  |
| 7   | CG    | 131 | LYS  |
| 10  | CJ    | 23  | ILE  |
| 10  | CJ    | 30  | SER  |
| 10  | CJ    | 32  | ALA  |
| 13  | CM    | 36  | LYS  |
| 13  | CM    | 113 | PRO  |
| 15  | CO    | 25  | THR  |
| 15  | CO    | 26  | GLU  |
| 15  | CO    | 80  | ALA  |
| 15  | CO    | 84  | LYS  |
| 16  | CP    | 54  | GLU  |
| 18  | CR    | 87  | ARG  |
| 19  | CS    | 30  | LEU  |
| 19  | CS    | 42  | PRO  |
| 19  | CS    | 50  | ALA  |
| 20  | CT    | 34  | LYS  |
| 20  | CT    | 78  | ALA  |
| 20  | CT    | 96  | GLY  |
| 20  | CT    | 98  | PRO  |
| 21  | CU    | 25  | LYS  |
| 24  | CY    | 88  | VAL  |
| 24  | CY    | 137 | ASN  |
| 24  | CY    | 174 | PHE  |
| 24  | CY    | 227 | ILE  |
| 24  | CY    | 371 | ALA  |
| 24  | CY    | 419 | ALA  |
| 24  | CY    | 427 | ALA  |
| 24  | CY    | 470 | PHE  |
| 24  | CY    | 559 | PRO  |
| 25  | D0    | 42  | GLY  |
| 26  | D1    | 24  | ALA  |
| 27  | D2    | 18  | PRO  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | D3    | 38  | GLU  |
| 31  | D6    | 41  | PRO  |
| 33  | D8    | 3   | LYS  |
| 33  | D8    | 61  | LEU  |
| 37  | DC    | 168 | LYS  |
| 37  | DC    | 227 | PRO  |
| 39  | DE    | 17  | ASP  |
| 39  | DE    | 45  | THR  |
| 39  | DE    | 64  | LYS  |
| 39  | DE    | 70  | ALA  |
| 39  | DE    | 117 | MET  |
| 40  | DF    | 90  | PHE  |
| 40  | DF    | 122 | LYS  |
| 40  | DF    | 134 | GLY  |
| 41  | DG    | 97  | ASP  |
| 41  | DG    | 140 | ILE  |
| 42  | DH    | 81  | GLU  |
| 44  | DK    | 116 | ASN  |
| 48  | DP    | 89  | ALA  |
| 48  | DP    | 106 | LEU  |
| 48  | DP    | 107 | LYS  |
| 49  | DQ    | 139 | GLU  |
| 50  | DR    | 31  | HIS  |
| 50  | DR    | 61  | HIS  |
| 51  | DS    | 15  | ARG  |
| 51  | DS    | 89  | ARG  |
| 51  | DS    | 105 | ALA  |
| 52  | DT    | 3   | ARG  |
| 52  | DT    | 9   | LEU  |
| 52  | DT    | 103 | ARG  |
| 55  | DW    | 99  | ARG  |
| 57  | DY    | 67  | LEU  |
| 58  | DZ    | 41  | LEU  |
| 58  | DZ    | 120 | ILE  |
| 58  | DZ    | 165 | VAL  |
| 58  | DZ    | 169 | GLU  |
| 2   | AB    | 9   | GLU  |
| 2   | AB    | 84  | GLU  |
| 2   | AB    | 212 | GLN  |
| 3   | AC    | 35  | GLU  |
| 3   | AC    | 179 | ARG  |
| 4   | AD    | 149 | ALA  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | AD    | 159 | ARG  |
| 4   | AD    | 186 | LEU  |
| 6   | AF    | 21  | LEU  |
| 8   | AH    | 121 | ASP  |
| 9   | AI    | 94  | ALA  |
| 9   | AI    | 106 | ALA  |
| 10  | AJ    | 30  | SER  |
| 10  | AJ    | 91  | PRO  |
| 11  | AK    | 34  | ASP  |
| 13  | AM    | 10  | PRO  |
| 15  | AO    | 25  | THR  |
| 16  | AP    | 54  | GLU  |
| 18  | AR    | 87  | ARG  |
| 19  | AS    | 30  | LEU  |
| 19  | AS    | 54  | GLY  |
| 19  | AS    | 59  | PRO  |
| 20  | AT    | 34  | LYS  |
| 20  | AT    | 44  | ALA  |
| 20  | AT    | 78  | ALA  |
| 20  | AT    | 104 | LEU  |
| 21  | AU    | 6   | ARG  |
| 24  | AY    | 22  | ASP  |
| 24  | AY    | 65  | ILE  |
| 24  | AY    | 123 | ARG  |
| 24  | AY    | 153 | MET  |
| 24  | AY    | 303 | PRO  |
| 24  | AY    | 361 | ASN  |
| 24  | AY    | 415 | PRO  |
| 24  | AY    | 577 | SER  |
| 24  | AY    | 598 | ASP  |
| 24  | AY    | 617 | MET  |
| 24  | AY    | 652 | MET  |
| 24  | AY    | 688 | ILE  |
| 26  | B1    | 30  | VAL  |
| 26  | B1    | 31  | GLY  |
| 27  | B2    | 14  | ARG  |
| 28  | B3    | 38  | GLU  |
| 29  | B4    | 2   | LYS  |
| 29  | B4    | 40  | HIS  |
| 30  | B5    | 4   | HIS  |
| 33  | B8    | 48  | PHE  |
| 33  | B8    | 61  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | BD    | 10  | THR  |
| 38  | BD    | 273 | ARG  |
| 39  | BE    | 45  | THR  |
| 39  | BE    | 187 | ALA  |
| 40  | BF    | 90  | PHE  |
| 41  | BG    | 106 | LEU  |
| 42  | BH    | 14  | GLY  |
| 42  | BH    | 81  | GLU  |
| 42  | BH    | 93  | GLY  |
| 46  | BN    | 127 | ASP  |
| 46  | BN    | 134 | ARG  |
| 48  | BP    | 23  | PRO  |
| 48  | BP    | 33  | ARG  |
| 48  | BP    | 83  | VAL  |
| 50  | BR    | 42  | LYS  |
| 50  | BR    | 102 | GLU  |
| 52  | BT    | 9   | LEU  |
| 52  | BT    | 17  | THR  |
| 53  | BU    | 46  | ALA  |
| 54  | BV    | 22  | VAL  |
| 55  | BW    | 93  | ALA  |
| 55  | BW    | 99  | ARG  |
| 56  | BX    | 11  | PRO  |
| 56  | BX    | 13  | LEU  |
| 57  | BY    | 37  | VAL  |
| 58  | BZ    | 46  | LYS  |
| 2   | CB    | 9   | GLU  |
| 2   | CB    | 84  | GLU  |
| 3   | CC    | 35  | GLU  |
| 3   | CC    | 44  | GLU  |
| 4   | CD    | 159 | ARG  |
| 4   | CD    | 186 | LEU  |
| 5   | CE    | 118 | ILE  |
| 6   | CF    | 21  | LEU  |
| 7   | CG    | 42  | ILE  |
| 8   | CH    | 121 | ASP  |
| 9   | CI    | 94  | ALA  |
| 10  | CJ    | 91  | PRO  |
| 11  | CK    | 34  | ASP  |
| 11  | CK    | 57  | THR  |
| 11  | CK    | 95  | ILE  |
| 12  | CL    | 19  | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | CM    | 10  | PRO  |
| 17  | CQ    | 25  | ARG  |
| 19  | CS    | 54  | GLY  |
| 19  | CS    | 59  | PRO  |
| 20  | CT    | 85  | MET  |
| 20  | CT    | 104 | LEU  |
| 21  | CU    | 6   | ARG  |
| 24  | CY    | 36  | THR  |
| 24  | CY    | 205 | TYR  |
| 24  | CY    | 206 | LEU  |
| 24  | CY    | 262 | SER  |
| 24  | CY    | 283 | PRO  |
| 24  | CY    | 315 | LYS  |
| 24  | CY    | 405 | PRO  |
| 26  | D1    | 63  | ALA  |
| 29  | D4    | 2   | LYS  |
| 29  | D4    | 40  | HIS  |
| 30  | D5    | 4   | HIS  |
| 33  | D8    | 48  | PHE  |
| 34  | D9    | 30  | PRO  |
| 38  | DD    | 10  | THR  |
| 38  | DD    | 273 | ARG  |
| 39  | DE    | 187 | ALA  |
| 40  | DF    | 62  | ARG  |
| 40  | DF    | 180 | GLY  |
| 41  | DG    | 12  | TYR  |
| 41  | DG    | 42  | GLY  |
| 42  | DH    | 111 | HIS  |
| 46  | DN    | 127 | ASP  |
| 46  | DN    | 134 | ARG  |
| 48  | DP    | 23  | PRO  |
| 48  | DP    | 33  | ARG  |
| 48  | DP    | 83  | VAL  |
| 48  | DP    | 108 | LYS  |
| 48  | DP    | 119 | GLU  |
| 50  | DR    | 86  | ARG  |
| 50  | DR    | 102 | GLU  |
| 52  | DT    | 17  | THR  |
| 52  | DT    | 26  | ASP  |
| 54  | DV    | 22  | VAL  |
| 55  | DW    | 111 | HIS  |
| 56  | DX    | 11  | PRO  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 56  | DX    | 13  | LEU  |
| 57  | DY    | 37  | VAL  |
| 58  | DZ    | 110 | GLY  |
| 2   | AB    | 157 | ARG  |
| 3   | AC    | 165 | THR  |
| 5   | AE    | 146 | ALA  |
| 9   | AI    | 127 | LYS  |
| 11  | AK    | 57  | THR  |
| 11  | AK    | 95  | ILE  |
| 13  | AM    | 21  | TYR  |
| 13  | AM    | 106 | ASN  |
| 17  | AQ    | 25  | ARG  |
| 24  | AY    | 24  | GLY  |
| 24  | AY    | 75  | LYS  |
| 24  | AY    | 408 | VAL  |
| 24  | AY    | 591 | LYS  |
| 25  | B0    | 13  | GLY  |
| 25  | B0    | 42  | GLY  |
| 27  | B2    | 44  | LEU  |
| 28  | B3    | 45  | GLY  |
| 31  | B6    | 36  | LEU  |
| 39  | BE    | 52  | LEU  |
| 39  | BE    | 73  | GLU  |
| 39  | BE    | 130 | GLY  |
| 40  | BF    | 14  | PRO  |
| 40  | BF    | 66  | PRO  |
| 42  | BH    | 48  | GLY  |
| 42  | BH    | 92  | ILE  |
| 42  | BH    | 111 | HIS  |
| 44  | BK    | 21  | PRO  |
| 44  | BK    | 73  | PRO  |
| 46  | BN    | 65  | LYS  |
| 46  | BN    | 81  | GLY  |
| 47  | BO    | 18  | LYS  |
| 48  | BP    | 141 | ALA  |
| 52  | BT    | 81  | PRO  |
| 55  | BW    | 14  | PRO  |
| 55  | BW    | 25  | ARG  |
| 2   | CB    | 157 | ARG  |
| 2   | CB    | 204 | ASN  |
| 3   | CC    | 160 | ALA  |
| 3   | CC    | 165 | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | CD    | 71  | SER  |
| 4   | CD    | 88  | VAL  |
| 8   | CH    | 135 | CYS  |
| 12  | CL    | 106 | ASP  |
| 13  | CM    | 116 | THR  |
| 20  | CT    | 44  | ALA  |
| 21  | CU    | 9   | ARG  |
| 24  | CY    | 408 | VAL  |
| 24  | CY    | 671 | MET  |
| 25  | D0    | 13  | GLY  |
| 26  | D1    | 52  | ARG  |
| 26  | D1    | 73  | LEU  |
| 39  | DE    | 73  | GLU  |
| 39  | DE    | 130 | GLY  |
| 40  | DF    | 2   | LYS  |
| 40  | DF    | 14  | PRO  |
| 40  | DF    | 66  | PRO  |
| 40  | DF    | 85  | GLY  |
| 41  | DG    | 22  | ARG  |
| 42  | DH    | 14  | GLY  |
| 42  | DH    | 45  | VAL  |
| 42  | DH    | 48  | GLY  |
| 42  | DH    | 92  | ILE  |
| 42  | DH    | 93  | GLY  |
| 44  | DK    | 21  | PRO  |
| 44  | DK    | 73  | PRO  |
| 46  | DN    | 65  | LYS  |
| 46  | DN    | 81  | GLY  |
| 47  | DO    | 18  | LYS  |
| 48  | DP    | 67  | MET  |
| 48  | DP    | 141 | ALA  |
| 49  | DQ    | 30  | GLY  |
| 50  | DR    | 42  | LYS  |
| 52  | DT    | 127 | ALA  |
| 53  | DU    | 46  | ALA  |
| 55  | DW    | 14  | PRO  |
| 55  | DW    | 25  | ARG  |
| 58  | DZ    | 12  | GLY  |
| 58  | DZ    | 65  | GLN  |
| 58  | DZ    | 121 | HIS  |
| 4   | AD    | 88  | VAL  |
| 5   | AE    | 118 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | AG    | 42  | ILE  |
| 9   | AI    | 74  | ILE  |
| 15  | AO    | 75  | PRO  |
| 26  | B1    | 87  | PRO  |
| 29  | B4    | 28  | LYS  |
| 40  | BF    | 177 | ALA  |
| 42  | BH    | 45  | VAL  |
| 42  | BH    | 76  | VAL  |
| 46  | BN    | 5   | VAL  |
| 49  | BQ    | 30  | GLY  |
| 52  | BT    | 92  | GLY  |
| 54  | BV    | 54  | GLY  |
| 55  | BW    | 59  | VAL  |
| 57  | BY    | 3   | VAL  |
| 9   | CI    | 74  | ILE  |
| 16  | CP    | 2   | VAL  |
| 19  | CS    | 51  | VAL  |
| 24  | CY    | 479 | PRO  |
| 24  | CY    | 670 | VAL  |
| 28  | D3    | 45  | GLY  |
| 29  | D4    | 28  | LYS  |
| 34  | D9    | 21  | GLY  |
| 39  | DE    | 52  | LEU  |
| 42  | DH    | 76  | VAL  |
| 52  | DT    | 81  | PRO  |
| 55  | DW    | 59  | VAL  |
| 2   | AB    | 26  | PRO  |
| 2   | AB    | 131 | PRO  |
| 2   | AB    | 232 | PRO  |
| 6   | AF    | 51  | PRO  |
| 7   | AG    | 9   | VAL  |
| 9   | AI    | 80  | GLY  |
| 16  | AP    | 2   | VAL  |
| 19  | AS    | 51  | VAL  |
| 26  | B1    | 36  | GLY  |
| 37  | BC    | 160 | GLY  |
| 38  | BD    | 228 | PRO  |
| 40  | BF    | 25  | PRO  |
| 40  | BF    | 85  | GLY  |
| 42  | BH    | 39  | PRO  |
| 48  | BP    | 146 | VAL  |
| 53  | BU    | 90  | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | BV    | 36  | PRO  |
| 57  | BY    | 31  | LEU  |
| 58  | BZ    | 134 | PRO  |
| 2   | CB    | 232 | PRO  |
| 6   | CF    | 51  | PRO  |
| 7   | CG    | 9   | VAL  |
| 7   | CG    | 82  | GLY  |
| 15  | CO    | 75  | PRO  |
| 24  | CY    | 554 | PRO  |
| 37  | DC    | 160 | GLY  |
| 40  | DF    | 25  | PRO  |
| 40  | DF    | 177 | ALA  |
| 46  | DN    | 5   | VAL  |
| 48  | DP    | 146 | VAL  |
| 53  | DU    | 90  | VAL  |
| 54  | DV    | 36  | PRO  |
| 54  | DV    | 54  | GLY  |
| 57  | DY    | 3   | VAL  |
| 57  | DY    | 31  | LEU  |
| 2   | AB    | 230 | VAL  |
| 7   | AG    | 82  | GLY  |
| 16  | AP    | 62  | VAL  |
| 20  | AT    | 100 | ILE  |
| 27  | B2    | 41  | ILE  |
| 37  | BC    | 68  | GLY  |
| 41  | BG    | 129 | GLY  |
| 51  | BS    | 22  | GLY  |
| 57  | BY    | 30  | VAL  |
| 58  | BZ    | 133 | ILE  |
| 2   | CB    | 131 | PRO  |
| 2   | CB    | 230 | VAL  |
| 9   | CI    | 80  | GLY  |
| 16  | CP    | 62  | VAL  |
| 20  | CT    | 100 | ILE  |
| 24  | CY    | 394 | ALA  |
| 24  | CY    | 600 | VAL  |
| 38  | DD    | 228 | PRO  |
| 39  | DE    | 34  | VAL  |
| 42  | DH    | 39  | PRO  |
| 51  | DS    | 22  | GLY  |
| 52  | DT    | 92  | GLY  |
| 53  | DU    | 9   | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 127 | ILE  |
| 2   | AB    | 194 | PRO  |
| 4   | AD    | 92  | VAL  |
| 4   | AD    | 180 | GLY  |
| 19  | AS    | 9   | VAL  |
| 26  | B1    | 86  | SER  |
| 37  | BC    | 136 | GLY  |
| 39  | BE    | 14  | ILE  |
| 39  | BE    | 34  | VAL  |
| 41  | BG    | 24  | GLY  |
| 42  | BH    | 107 | VAL  |
| 52  | BT    | 15  | VAL  |
| 54  | BV    | 51  | VAL  |
| 2   | CB    | 127 | ILE  |
| 2   | CB    | 194 | PRO  |
| 4   | CD    | 92  | VAL  |
| 14  | CN    | 55  | GLY  |
| 15  | CO    | 19  | PRO  |
| 24  | CY    | 532 | GLY  |
| 37  | DC    | 68  | GLY  |
| 37  | DC    | 101 | ILE  |
| 37  | DC    | 107 | GLY  |
| 37  | DC    | 136 | GLY  |
| 39  | DE    | 75  | VAL  |
| 51  | DS    | 91  | PRO  |
| 57  | DY    | 30  | VAL  |
| 58  | DZ    | 166 | SER  |
| 24  | AY    | 333 | GLY  |
| 37  | BC    | 107 | GLY  |
| 39  | BE    | 75  | VAL  |
| 42  | BH    | 52  | VAL  |
| 51  | BS    | 91  | PRO  |
| 57  | BY    | 27  | VAL  |
| 2   | CB    | 26  | PRO  |
| 24  | CY    | 293 | THR  |
| 30  | D5    | 50  | GLY  |
| 38  | DD    | 11  | PRO  |
| 39  | DE    | 14  | ILE  |
| 41  | DG    | 20  | ILE  |
| 42  | DH    | 52  | VAL  |
| 42  | DH    | 107 | VAL  |
| 52  | DT    | 15  | VAL  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | DV    | 51  | VAL  |
| 58  | DZ    | 14  | LYS  |
| 58  | DZ    | 134 | PRO  |
| 38  | BD    | 245 | PRO  |
| 38  | DD    | 245 | PRO  |

### 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   | AB    | 202/220 (92%)  | 179 (89%) | 23 (11%) | 7           | 35 |
| 2   | CB    | 202/220 (92%)  | 179 (89%) | 23 (11%) | 7           | 35 |
| 3   | AC    | 160/188 (85%)  | 142 (89%) | 18 (11%) | 7           | 35 |
| 3   | CC    | 160/188 (85%)  | 142 (89%) | 18 (11%) | 7           | 35 |
| 4   | AD    | 180/181 (99%)  | 160 (89%) | 20 (11%) | 7           | 37 |
| 4   | CD    | 180/181 (99%)  | 160 (89%) | 20 (11%) | 7           | 37 |
| 5   | AE    | 115/123 (94%)  | 100 (87%) | 15 (13%) | 5           | 29 |
| 5   | CE    | 115/123 (94%)  | 100 (87%) | 15 (13%) | 5           | 29 |
| 6   | AF    | 90/90 (100%)   | 83 (92%)  | 7 (8%)   | 15          | 51 |
| 6   | CF    | 90/90 (100%)   | 83 (92%)  | 7 (8%)   | 15          | 51 |
| 7   | AG    | 126/127 (99%)  | 117 (93%) | 9 (7%)   | 17          | 55 |
| 7   | CG    | 126/127 (99%)  | 117 (93%) | 9 (7%)   | 17          | 55 |
| 8   | AH    | 119/119 (100%) | 110 (92%) | 9 (8%)   | 15          | 52 |
| 8   | CH    | 119/119 (100%) | 112 (94%) | 7 (6%)   | 23          | 62 |
| 9   | AI    | 98/99 (99%)    | 90 (92%)  | 8 (8%)   | 13          | 49 |
| 9   | CI    | 98/99 (99%)    | 90 (92%)  | 8 (8%)   | 13          | 49 |
| 10  | AJ    | 88/92 (96%)    | 77 (88%)  | 11 (12%) | 5           | 31 |
| 10  | CJ    | 88/92 (96%)    | 77 (88%)  | 11 (12%) | 5           | 31 |
| 11  | AK    | 90/99 (91%)    | 84 (93%)  | 6 (7%)   | 19          | 58 |
| 11  | CK    | 90/99 (91%)    | 84 (93%)  | 6 (7%)   | 19          | 58 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|-------------|-----|
| 12  | AL    | 104/109 (95%) | 94 (90%)  | 10 (10%) | 10          | 43  |
| 12  | CL    | 104/109 (95%) | 93 (89%)  | 11 (11%) | 8           | 38  |
| 13  | AM    | 99/101 (98%)  | 91 (92%)  | 8 (8%)   | 14          | 50  |
| 13  | CM    | 99/101 (98%)  | 91 (92%)  | 8 (8%)   | 14          | 50  |
| 14  | AN    | 49/50 (98%)   | 43 (88%)  | 6 (12%)  | 6           | 31  |
| 14  | CN    | 49/50 (98%)   | 43 (88%)  | 6 (12%)  | 6           | 31  |
| 15  | AO    | 79/80 (99%)   | 71 (90%)  | 8 (10%)  | 9           | 40  |
| 15  | CO    | 79/80 (99%)   | 71 (90%)  | 8 (10%)  | 9           | 40  |
| 16  | AP    | 72/74 (97%)   | 67 (93%)  | 5 (7%)   | 18          | 56  |
| 16  | CP    | 72/74 (97%)   | 67 (93%)  | 5 (7%)   | 18          | 56  |
| 17  | AQ    | 94/97 (97%)   | 87 (93%)  | 7 (7%)   | 16          | 53  |
| 17  | CQ    | 94/97 (97%)   | 87 (93%)  | 7 (7%)   | 16          | 53  |
| 18  | AR    | 61/77 (79%)   | 59 (97%)  | 2 (3%)   | 43          | 77  |
| 18  | CR    | 61/77 (79%)   | 59 (97%)  | 2 (3%)   | 43          | 77  |
| 19  | AS    | 69/80 (86%)   | 59 (86%)  | 10 (14%) | 4           | 25  |
| 19  | CS    | 69/80 (86%)   | 59 (86%)  | 10 (14%) | 4           | 25  |
| 20  | AT    | 76/82 (93%)   | 69 (91%)  | 7 (9%)   | 11          | 45  |
| 20  | CT    | 76/82 (93%)   | 69 (91%)  | 7 (9%)   | 11          | 45  |
| 21  | AU    | 19/22 (86%)   | 19 (100%) | 0        | 100         | 100 |
| 21  | CU    | 19/22 (86%)   | 19 (100%) | 0        | 100         | 100 |
| 24  | AY    | 563/582 (97%) | 489 (87%) | 74 (13%) | 5           | 29  |
| 24  | CY    | 563/582 (97%) | 495 (88%) | 68 (12%) | 6           | 32  |
| 25  | B0    | 66/67 (98%)   | 57 (86%)  | 9 (14%)  | 4           | 28  |
| 25  | D0    | 66/67 (98%)   | 57 (86%)  | 9 (14%)  | 4           | 28  |
| 26  | B1    | 78/83 (94%)   | 65 (83%)  | 13 (17%) | 2           | 17  |
| 26  | D1    | 78/83 (94%)   | 70 (90%)  | 8 (10%)  | 8           | 40  |
| 27  | B2    | 66/67 (98%)   | 59 (89%)  | 7 (11%)  | 8           | 38  |
| 27  | D2    | 66/67 (98%)   | 58 (88%)  | 8 (12%)  | 6           | 32  |
| 28  | B3    | 51/52 (98%)   | 47 (92%)  | 4 (8%)   | 15          | 51  |
| 28  | D3    | 51/52 (98%)   | 47 (92%)  | 4 (8%)   | 15          | 51  |
| 29  | B4    | 51/63 (81%)   | 38 (74%)  | 13 (26%) | 0           | 5   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 29  | D4    | 51/63 (81%)    | 37 (72%)  | 14 (28%) | 0           | 4  |
| 30  | B5    | 51/52 (98%)    | 45 (88%)  | 6 (12%)  | 6           | 33 |
| 30  | D5    | 51/52 (98%)    | 45 (88%)  | 6 (12%)  | 6           | 33 |
| 31  | B6    | 49/52 (94%)    | 39 (80%)  | 10 (20%) | 1           | 10 |
| 31  | D6    | 49/52 (94%)    | 38 (78%)  | 11 (22%) | 1           | 7  |
| 32  | B7    | 41/42 (98%)    | 36 (88%)  | 5 (12%)  | 6           | 31 |
| 32  | D7    | 41/42 (98%)    | 36 (88%)  | 5 (12%)  | 6           | 31 |
| 33  | B8    | 53/55 (96%)    | 44 (83%)  | 9 (17%)  | 2           | 17 |
| 33  | D8    | 53/55 (96%)    | 43 (81%)  | 10 (19%) | 2           | 11 |
| 34  | B9    | 34/34 (100%)   | 30 (88%)  | 4 (12%)  | 6           | 33 |
| 34  | D9    | 34/34 (100%)   | 29 (85%)  | 5 (15%)  | 3           | 24 |
| 37  | BC    | 180/181 (99%)  | 170 (94%) | 10 (6%)  | 25          | 63 |
| 37  | DC    | 180/181 (99%)  | 169 (94%) | 11 (6%)  | 22          | 61 |
| 38  | BD    | 217/218 (100%) | 177 (82%) | 40 (18%) | 2           | 12 |
| 38  | DD    | 217/218 (100%) | 178 (82%) | 39 (18%) | 2           | 13 |
| 39  | BE    | 165/166 (99%)  | 139 (84%) | 26 (16%) | 3           | 21 |
| 39  | DE    | 165/166 (99%)  | 140 (85%) | 25 (15%) | 3           | 22 |
| 40  | BF    | 165/166 (99%)  | 153 (93%) | 12 (7%)  | 16          | 54 |
| 40  | DF    | 165/166 (99%)  | 153 (93%) | 12 (7%)  | 16          | 54 |
| 41  | BG    | 155/156 (99%)  | 131 (84%) | 24 (16%) | 3           | 21 |
| 41  | DG    | 155/156 (99%)  | 126 (81%) | 29 (19%) | 2           | 12 |
| 42  | BH    | 136/148 (92%)  | 126 (93%) | 10 (7%)  | 16          | 53 |
| 42  | DH    | 136/148 (92%)  | 126 (93%) | 10 (7%)  | 16          | 53 |
| 44  | BK    | 104/111 (94%)  | 89 (86%)  | 15 (14%) | 4           | 25 |
| 44  | DK    | 104/111 (94%)  | 90 (86%)  | 14 (14%) | 4           | 28 |
| 46  | BN    | 117/119 (98%)  | 103 (88%) | 14 (12%) | 6           | 32 |
| 46  | DN    | 117/119 (98%)  | 102 (87%) | 15 (13%) | 5           | 29 |
| 47  | BO    | 100/100 (100%) | 92 (92%)  | 8 (8%)   | 14          | 50 |
| 47  | DO    | 100/100 (100%) | 92 (92%)  | 8 (8%)   | 14          | 50 |
| 48  | BP    | 112/116 (97%)  | 91 (81%)  | 21 (19%) | 2           | 12 |
| 48  | DP    | 112/116 (97%)  | 91 (81%)  | 21 (19%) | 2           | 12 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed          | Rotameric  | Outliers   | Percentiles |    |
|-----|-------|-------------------|------------|------------|-------------|----|
| 49  | BQ    | 111/111 (100%)    | 95 (86%)   | 16 (14%)   | 4           | 25 |
| 49  | DQ    | 111/111 (100%)    | 97 (87%)   | 14 (13%)   | 5           | 30 |
| 50  | BR    | 100/101 (99%)     | 89 (89%)   | 11 (11%)   | 7           | 37 |
| 50  | DR    | 100/101 (99%)     | 88 (88%)   | 12 (12%)   | 6           | 32 |
| 51  | BS    | 77/88 (88%)       | 68 (88%)   | 9 (12%)    | 6           | 34 |
| 51  | DS    | 77/88 (88%)       | 68 (88%)   | 9 (12%)    | 6           | 34 |
| 52  | BT    | 120/127 (94%)     | 97 (81%)   | 23 (19%)   | 1           | 11 |
| 52  | DT    | 120/127 (94%)     | 97 (81%)   | 23 (19%)   | 1           | 11 |
| 53  | BU    | 92/94 (98%)       | 83 (90%)   | 9 (10%)    | 9           | 42 |
| 53  | DU    | 92/94 (98%)       | 83 (90%)   | 9 (10%)    | 9           | 42 |
| 54  | BV    | 82/82 (100%)      | 71 (87%)   | 11 (13%)   | 4           | 28 |
| 54  | DV    | 82/82 (100%)      | 71 (87%)   | 11 (13%)   | 4           | 28 |
| 55  | BW    | 91/92 (99%)       | 84 (92%)   | 7 (8%)     | 15          | 52 |
| 55  | DW    | 91/92 (99%)       | 84 (92%)   | 7 (8%)     | 15          | 52 |
| 56  | BX    | 74/78 (95%)       | 64 (86%)   | 10 (14%)   | 4           | 28 |
| 56  | DX    | 74/78 (95%)       | 64 (86%)   | 10 (14%)   | 4           | 28 |
| 57  | BY    | 87/91 (96%)       | 75 (86%)   | 12 (14%)   | 4           | 27 |
| 57  | DY    | 87/91 (96%)       | 75 (86%)   | 12 (14%)   | 4           | 27 |
| 58  | BZ    | 162/179 (90%)     | 134 (83%)  | 28 (17%)   | 2           | 15 |
| 58  | DZ    | 162/179 (90%)     | 144 (89%)  | 18 (11%)   | 7           | 37 |
| All | All   | 11080/11566 (96%) | 9776 (88%) | 1304 (12%) | 6           | 33 |

All (1304) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 15  | VAL  |
| 2   | AB    | 16  | HIS  |
| 2   | AB    | 17  | PHE  |
| 2   | AB    | 24  | TRP  |
| 2   | AB    | 36  | ARG  |
| 2   | AB    | 43  | ASP  |
| 2   | AB    | 44  | LEU  |
| 2   | AB    | 67  | THR  |
| 2   | AB    | 79  | ASP  |
| 2   | AB    | 101 | MET  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 111 | ARG  |
| 2   | AB    | 129 | GLU  |
| 2   | AB    | 137 | ARG  |
| 2   | AB    | 157 | ARG  |
| 2   | AB    | 162 | ILE  |
| 2   | AB    | 172 | ILE  |
| 2   | AB    | 178 | ARG  |
| 2   | AB    | 192 | SER  |
| 2   | AB    | 200 | ILE  |
| 2   | AB    | 204 | ASN  |
| 2   | AB    | 212 | GLN  |
| 2   | AB    | 220 | ASP  |
| 2   | AB    | 221 | LEU  |
| 3   | AC    | 5   | ILE  |
| 3   | AC    | 16  | ARG  |
| 3   | AC    | 29  | TYR  |
| 3   | AC    | 34  | LEU  |
| 3   | AC    | 56  | ASP  |
| 3   | AC    | 72  | LYS  |
| 3   | AC    | 79  | ARG  |
| 3   | AC    | 85  | ARG  |
| 3   | AC    | 95  | THR  |
| 3   | AC    | 98  | ASN  |
| 3   | AC    | 125 | GLU  |
| 3   | AC    | 127 | ARG  |
| 3   | AC    | 152 | ILE  |
| 3   | AC    | 156 | ARG  |
| 3   | AC    | 165 | THR  |
| 3   | AC    | 167 | TRP  |
| 3   | AC    | 178 | LEU  |
| 3   | AC    | 179 | ARG  |
| 4   | AD    | 3   | ARG  |
| 4   | AD    | 9   | CYS  |
| 4   | AD    | 12  | CYS  |
| 4   | AD    | 15  | GLU  |
| 4   | AD    | 22  | LYS  |
| 4   | AD    | 36  | ARG  |
| 4   | AD    | 49  | ARG  |
| 4   | AD    | 53  | ASP  |
| 4   | AD    | 57  | ARG  |
| 4   | AD    | 70  | ILE  |
| 4   | AD    | 73  | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | AD    | 78  | LEU  |
| 4   | AD    | 96  | LEU  |
| 4   | AD    | 114 | ARG  |
| 4   | AD    | 127 | THR  |
| 4   | AD    | 131 | ARG  |
| 4   | AD    | 132 | ARG  |
| 4   | AD    | 135 | LEU  |
| 4   | AD    | 162 | LEU  |
| 4   | AD    | 168 | ARG  |
| 5   | AE    | 12  | LEU  |
| 5   | AE    | 18  | ARG  |
| 5   | AE    | 20  | GLN  |
| 5   | AE    | 31  | LEU  |
| 5   | AE    | 41  | VAL  |
| 5   | AE    | 47  | LYS  |
| 5   | AE    | 56  | GLN  |
| 5   | AE    | 64  | ARG  |
| 5   | AE    | 72  | GLN  |
| 5   | AE    | 75  | THR  |
| 5   | AE    | 76  | ILE  |
| 5   | AE    | 79  | GLU  |
| 5   | AE    | 101 | ILE  |
| 5   | AE    | 117 | ASP  |
| 5   | AE    | 144 | THR  |
| 6   | AF    | 15  | ASP  |
| 6   | AF    | 32  | ASN  |
| 6   | AF    | 43  | LEU  |
| 6   | AF    | 47  | ARG  |
| 6   | AF    | 69  | GLU  |
| 6   | AF    | 86  | ARG  |
| 6   | AF    | 98  | LEU  |
| 7   | AG    | 27  | ILE  |
| 7   | AG    | 57  | GLU  |
| 7   | AG    | 66  | VAL  |
| 7   | AG    | 79  | ARG  |
| 7   | AG    | 104 | LEU  |
| 7   | AG    | 113 | GLU  |
| 7   | AG    | 124 | LEU  |
| 7   | AG    | 137 | LYS  |
| 7   | AG    | 151 | TYR  |
| 8   | AH    | 1   | MET  |
| 8   | AH    | 25  | ASP  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | AH    | 54  | ASP  |
| 8   | AH    | 83  | ILE  |
| 8   | AH    | 91  | ARG  |
| 8   | AH    | 92  | ARG  |
| 8   | AH    | 98  | LYS  |
| 8   | AH    | 102 | ARG  |
| 8   | AH    | 118 | VAL  |
| 9   | AI    | 4   | TYR  |
| 9   | AI    | 10  | ARG  |
| 9   | AI    | 29  | ASN  |
| 9   | AI    | 59  | PHE  |
| 9   | AI    | 95  | LYS  |
| 9   | AI    | 114 | TYR  |
| 9   | AI    | 121 | ARG  |
| 9   | AI    | 128 | ARG  |
| 10  | AJ    | 22  | LYS  |
| 10  | AJ    | 40  | LEU  |
| 10  | AJ    | 43  | ARG  |
| 10  | AJ    | 50  | ILE  |
| 10  | AJ    | 55  | LYS  |
| 10  | AJ    | 59  | SER  |
| 10  | AJ    | 62  | HIS  |
| 10  | AJ    | 63  | PHE  |
| 10  | AJ    | 74  | ILE  |
| 10  | AJ    | 76  | ASN  |
| 10  | AJ    | 96  | ILE  |
| 11  | AK    | 29  | ILE  |
| 11  | AK    | 87  | THR  |
| 11  | AK    | 91  | ARG  |
| 11  | AK    | 92  | GLU  |
| 11  | AK    | 117 | ASN  |
| 11  | AK    | 124 | LYS  |
| 12  | AL    | 7   | ILE  |
| 12  | AL    | 20  | LYS  |
| 12  | AL    | 38  | THR  |
| 12  | AL    | 41  | ARG  |
| 12  | AL    | 47  | LYS  |
| 12  | AL    | 53  | ARG  |
| 12  | AL    | 70  | ILE  |
| 12  | AL    | 81  | SER  |
| 12  | AL    | 85  | ILE  |
| 12  | AL    | 113 | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | AM    | 64  | TRP  |
| 13  | AM    | 66  | LEU  |
| 13  | AM    | 108 | ARG  |
| 13  | AM    | 113 | PRO  |
| 13  | AM    | 115 | LYS  |
| 13  | AM    | 120 | LYS  |
| 13  | AM    | 121 | LYS  |
| 13  | AM    | 124 | PRO  |
| 14  | AN    | 14  | PRO  |
| 14  | AN    | 16  | PHE  |
| 14  | AN    | 29  | ARG  |
| 14  | AN    | 41  | ARG  |
| 14  | AN    | 42  | ILE  |
| 14  | AN    | 44  | LEU  |
| 15  | AO    | 10  | LYS  |
| 15  | AO    | 39  | LEU  |
| 15  | AO    | 41  | GLU  |
| 15  | AO    | 57  | LEU  |
| 15  | AO    | 65  | ARG  |
| 15  | AO    | 82  | ILE  |
| 15  | AO    | 85  | LEU  |
| 15  | AO    | 88  | ARG  |
| 16  | AP    | 1   | MET  |
| 16  | AP    | 2   | VAL  |
| 16  | AP    | 6   | LEU  |
| 16  | AP    | 11  | SER  |
| 16  | AP    | 32  | TYR  |
| 17  | AQ    | 7   | THR  |
| 17  | AQ    | 9   | VAL  |
| 17  | AQ    | 23  | VAL  |
| 17  | AQ    | 35  | VAL  |
| 17  | AQ    | 48  | GLU  |
| 17  | AQ    | 52  | LYS  |
| 17  | AQ    | 78  | GLU  |
| 18  | AR    | 29  | PHE  |
| 18  | AR    | 31  | LEU  |
| 19  | AS    | 5   | LEU  |
| 19  | AS    | 6   | LYS  |
| 19  | AS    | 7   | LYS  |
| 19  | AS    | 15  | LEU  |
| 19  | AS    | 19  | VAL  |
| 19  | AS    | 29  | ARG  |

*Continued on next page...*



*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 19         | AS           | 37         | ARG         |
| 19         | AS           | 44         | MET         |
| 19         | AS           | 66         | MET         |
| 19         | AS           | 77         | THR         |
| 20         | AT           | 13         | LEU         |
| 20         | AT           | 24         | LEU         |
| 20         | AT           | 26         | ASN         |
| 20         | AT           | 36         | LEU         |
| 20         | AT           | 74         | LYS         |
| 20         | AT           | 84         | LEU         |
| 20         | AT           | 93         | GLU         |
| 24         | AY           | 20         | HIS         |
| 24         | AY           | 21         | ILE         |
| 24         | AY           | 40         | HIS         |
| 24         | AY           | 65         | ILE         |
| 24         | AY           | 83         | ASP         |
| 24         | AY           | 85         | PRO         |
| 24         | AY           | 88         | VAL         |
| 24         | AY           | 89         | ASP         |
| 24         | AY           | 92         | ILE         |
| 24         | AY           | 96         | ARG         |
| 24         | AY           | 100        | VAL         |
| 24         | AY           | 101        | LEU         |
| 24         | AY           | 102        | ASP         |
| 24         | AY           | 111        | SER         |
| 24         | AY           | 117        | GLN         |
| 24         | AY           | 122        | TRP         |
| 24         | AY           | 124        | GLN         |
| 24         | AY           | 130        | VAL         |
| 24         | AY           | 132        | ARG         |
| 24         | AY           | 137        | ASN         |
| 24         | AY           | 152        | THR         |
| 24         | AY           | 157        | LEU         |
| 24         | AY           | 170        | ARG         |
| 24         | AY           | 191        | ASP         |
| 24         | AY           | 192        | LEU         |
| 24         | AY           | 240        | GLU         |
| 24         | AY           | 242        | LEU         |
| 24         | AY           | 252        | ASP         |
| 24         | AY           | 255        | ILE         |
| 24         | AY           | 260        | LEU         |
| 24         | AY           | 270        | GLN         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | AY    | 289 | ILE  |
| 24  | AY    | 298 | VAL  |
| 24  | AY    | 312 | LEU  |
| 24  | AY    | 319 | ASP  |
| 24  | AY    | 326 | THR  |
| 24  | AY    | 337 | SER  |
| 24  | AY    | 343 | ASN  |
| 24  | AY    | 357 | ARG  |
| 24  | AY    | 378 | VAL  |
| 24  | AY    | 381 | LYS  |
| 24  | AY    | 388 | THR  |
| 24  | AY    | 399 | LEU  |
| 24  | AY    | 409 | ILE  |
| 24  | AY    | 410 | ASP  |
| 24  | AY    | 420 | ASP  |
| 24  | AY    | 421 | GLN  |
| 24  | AY    | 426 | GLN  |
| 24  | AY    | 428 | LEU  |
| 24  | AY    | 438 | PHE  |
| 24  | AY    | 440 | VAL  |
| 24  | AY    | 468 | ARG  |
| 24  | AY    | 476 | VAL  |
| 24  | AY    | 481 | VAL  |
| 24  | AY    | 487 | ILE  |
| 24  | AY    | 501 | THR  |
| 24  | AY    | 504 | ARG  |
| 24  | AY    | 509 | HIS  |
| 24  | AY    | 512 | ILE  |
| 24  | AY    | 515 | GLU  |
| 24  | AY    | 525 | PHE  |
| 24  | AY    | 527 | ASN  |
| 24  | AY    | 567 | LEU  |
| 24  | AY    | 572 | TYR  |
| 24  | AY    | 574 | GLU  |
| 24  | AY    | 595 | GLN  |
| 24  | AY    | 598 | ASP  |
| 24  | AY    | 614 | GLU  |
| 24  | AY    | 630 | GLN  |
| 24  | AY    | 631 | ILE  |
| 24  | AY    | 634 | MET  |
| 24  | AY    | 644 | ARG  |
| 24  | AY    | 657 | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | AY    | 685 | GLU  |
| 25  | B0    | 5   | LYS  |
| 25  | B0    | 11  | ARG  |
| 25  | B0    | 20  | ARG  |
| 25  | B0    | 27  | GLU  |
| 25  | B0    | 41  | ARG  |
| 25  | B0    | 60  | PHE  |
| 25  | B0    | 75  | LEU  |
| 25  | B0    | 78  | TYR  |
| 25  | B0    | 84  | LEU  |
| 26  | B1    | 18  | ILE  |
| 26  | B1    | 35  | THR  |
| 26  | B1    | 45  | ASN  |
| 26  | B1    | 46  | LEU  |
| 26  | B1    | 56  | GLN  |
| 26  | B1    | 65  | SER  |
| 26  | B1    | 72  | GLU  |
| 26  | B1    | 73  | LEU  |
| 26  | B1    | 75  | GLU  |
| 26  | B1    | 80  | LEU  |
| 26  | B1    | 83  | GLU  |
| 26  | B1    | 94  | LEU  |
| 26  | B1    | 95  | LEU  |
| 27  | B2    | 3   | LEU  |
| 27  | B2    | 30  | ARG  |
| 27  | B2    | 32  | LEU  |
| 27  | B2    | 44  | LEU  |
| 27  | B2    | 52  | ASP  |
| 27  | B2    | 59  | ARG  |
| 27  | B2    | 64  | LEU  |
| 28  | B3    | 8   | LEU  |
| 28  | B3    | 28  | LEU  |
| 28  | B3    | 38  | GLU  |
| 28  | B3    | 48  | GLU  |
| 29  | B4    | 1   | MET  |
| 29  | B4    | 5   | ILE  |
| 29  | B4    | 8   | LYS  |
| 29  | B4    | 9   | LEU  |
| 29  | B4    | 13  | ARG  |
| 29  | B4    | 20  | ASN  |
| 29  | B4    | 32  | TYR  |
| 29  | B4    | 40  | HIS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | B4    | 42  | PHE  |
| 29  | B4    | 43  | TYR  |
| 29  | B4    | 49  | PHE  |
| 29  | B4    | 51  | ASP  |
| 29  | B4    | 55  | ARG  |
| 30  | B5    | 3   | LYS  |
| 30  | B5    | 4   | HIS  |
| 30  | B5    | 23  | HIS  |
| 30  | B5    | 36  | CYS  |
| 30  | B5    | 55  | ARG  |
| 30  | B5    | 58  | LEU  |
| 31  | B6    | 6   | ARG  |
| 31  | B6    | 9   | LEU  |
| 31  | B6    | 10  | LEU  |
| 31  | B6    | 11  | LEU  |
| 31  | B6    | 15  | GLU  |
| 31  | B6    | 23  | THR  |
| 31  | B6    | 30  | THR  |
| 31  | B6    | 31  | PRO  |
| 31  | B6    | 39  | TYR  |
| 31  | B6    | 42  | TRP  |
| 32  | B7    | 1   | MET  |
| 32  | B7    | 4   | THR  |
| 32  | B7    | 8   | ASN  |
| 32  | B7    | 41  | ARG  |
| 32  | B7    | 48  | LYS  |
| 33  | B8    | 6   | THR  |
| 33  | B8    | 30  | ARG  |
| 33  | B8    | 32  | LEU  |
| 33  | B8    | 33  | ASN  |
| 33  | B8    | 34  | TRP  |
| 33  | B8    | 44  | LYS  |
| 33  | B8    | 48  | PHE  |
| 33  | B8    | 49  | VAL  |
| 33  | B8    | 61  | LEU  |
| 34  | B9    | 1   | MET  |
| 34  | B9    | 10  | ILE  |
| 34  | B9    | 11  | CYS  |
| 34  | B9    | 29  | ASN  |
| 37  | BC    | 18  | ASN  |
| 37  | BC    | 53  | ARG  |
| 37  | BC    | 54  | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | BC    | 74  | ARG  |
| 37  | BC    | 149 | ASN  |
| 37  | BC    | 184 | GLU  |
| 37  | BC    | 185 | LYS  |
| 37  | BC    | 189 | ASN  |
| 37  | BC    | 191 | ARG  |
| 37  | BC    | 212 | SER  |
| 38  | BD    | 10  | THR  |
| 38  | BD    | 23  | GLU  |
| 38  | BD    | 24  | ILE  |
| 38  | BD    | 26  | LYS  |
| 38  | BD    | 35  | LYS  |
| 38  | BD    | 37  | LEU  |
| 38  | BD    | 43  | ARG  |
| 38  | BD    | 61  | LEU  |
| 38  | BD    | 63  | ARG  |
| 38  | BD    | 65  | ILE  |
| 38  | BD    | 87  | ASN  |
| 38  | BD    | 89  | SER  |
| 38  | BD    | 92  | ILE  |
| 38  | BD    | 94  | LEU  |
| 38  | BD    | 95  | LEU  |
| 38  | BD    | 96  | HIS  |
| 38  | BD    | 104 | TYR  |
| 38  | BD    | 106 | ILE  |
| 38  | BD    | 111 | LEU  |
| 38  | BD    | 117 | VAL  |
| 38  | BD    | 131 | LEU  |
| 38  | BD    | 157 | ARG  |
| 38  | BD    | 166 | GLN  |
| 38  | BD    | 183 | ARG  |
| 38  | BD    | 190 | TYR  |
| 38  | BD    | 192 | THR  |
| 38  | BD    | 202 | LYS  |
| 38  | BD    | 211 | ARG  |
| 38  | BD    | 212 | SER  |
| 38  | BD    | 221 | VAL  |
| 38  | BD    | 227 | ASN  |
| 38  | BD    | 228 | PRO  |
| 38  | BD    | 244 | ARG  |
| 38  | BD    | 246 | PRO  |
| 38  | BD    | 257 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | BD    | 260 | ARG  |
| 38  | BD    | 263 | ARG  |
| 38  | BD    | 270 | ILE  |
| 38  | BD    | 273 | ARG  |
| 38  | BD    | 275 | LYS  |
| 39  | BE    | 4   | ILE  |
| 39  | BE    | 9   | VAL  |
| 39  | BE    | 18  | ASP  |
| 39  | BE    | 24  | THR  |
| 39  | BE    | 36  | ARG  |
| 39  | BE    | 49  | LEU  |
| 39  | BE    | 54  | GLN  |
| 39  | BE    | 55  | ASN  |
| 39  | BE    | 61  | ARG  |
| 39  | BE    | 67  | PHE  |
| 39  | BE    | 69  | LYS  |
| 39  | BE    | 78  | LEU  |
| 39  | BE    | 79  | ARG  |
| 39  | BE    | 94  | GLU  |
| 39  | BE    | 95  | ILE  |
| 39  | BE    | 118 | LYS  |
| 39  | BE    | 119 | ARG  |
| 39  | BE    | 121 | ASN  |
| 39  | BE    | 134 | ILE  |
| 39  | BE    | 144 | ARG  |
| 39  | BE    | 178 | GLU  |
| 39  | BE    | 184 | VAL  |
| 39  | BE    | 192 | ASN  |
| 39  | BE    | 197 | ILE  |
| 39  | BE    | 202 | LYS  |
| 39  | BE    | 203 | LYS  |
| 40  | BF    | 19  | GLU  |
| 40  | BF    | 28  | ILE  |
| 40  | BF    | 41  | LEU  |
| 40  | BF    | 64  | ILE  |
| 40  | BF    | 66  | PRO  |
| 40  | BF    | 83  | PHE  |
| 40  | BF    | 125 | LEU  |
| 40  | BF    | 149 | ASP  |
| 40  | BF    | 160 | ASN  |
| 40  | BF    | 165 | ARG  |
| 40  | BF    | 175 | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | BF    | 179 | GLU  |
| 41  | BG    | 4   | ASP  |
| 41  | BG    | 5   | VAL  |
| 41  | BG    | 16  | ARG  |
| 41  | BG    | 22  | ARG  |
| 41  | BG    | 33  | ARG  |
| 41  | BG    | 34  | LEU  |
| 41  | BG    | 36  | LYS  |
| 41  | BG    | 60  | LEU  |
| 41  | BG    | 71  | THR  |
| 41  | BG    | 80  | PHE  |
| 41  | BG    | 83  | ARG  |
| 41  | BG    | 91  | ARG  |
| 41  | BG    | 98  | ARG  |
| 41  | BG    | 118 | ARG  |
| 41  | BG    | 128 | ARG  |
| 41  | BG    | 133 | LEU  |
| 41  | BG    | 135 | LEU  |
| 41  | BG    | 145 | THR  |
| 41  | BG    | 147 | ASP  |
| 41  | BG    | 148 | MET  |
| 41  | BG    | 152 | LEU  |
| 41  | BG    | 159 | VAL  |
| 41  | BG    | 164 | GLU  |
| 41  | BG    | 166 | ASP  |
| 42  | BH    | 46  | GLU  |
| 42  | BH    | 49  | VAL  |
| 42  | BH    | 53  | GLU  |
| 42  | BH    | 54  | ARG  |
| 42  | BH    | 83  | TYR  |
| 42  | BH    | 89  | ILE  |
| 42  | BH    | 104 | GLU  |
| 42  | BH    | 105 | LEU  |
| 42  | BH    | 143 | GLN  |
| 42  | BH    | 158 | HIS  |
| 44  | BK    | 2   | LYS  |
| 44  | BK    | 3   | LYS  |
| 44  | BK    | 5   | VAL  |
| 44  | BK    | 29  | GLN  |
| 44  | BK    | 30  | HIS  |
| 44  | BK    | 34  | ILE  |
| 44  | BK    | 38  | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44  | BK    | 47  | ASN  |
| 44  | BK    | 65  | PHE  |
| 44  | BK    | 70  | LYS  |
| 44  | BK    | 77  | LEU  |
| 44  | BK    | 86  | LYS  |
| 44  | BK    | 95  | LYS  |
| 44  | BK    | 105 | LEU  |
| 44  | BK    | 117 | THR  |
| 46  | BN    | 1   | MET  |
| 46  | BN    | 4   | TYR  |
| 46  | BN    | 23  | LEU  |
| 46  | BN    | 26  | LEU  |
| 46  | BN    | 39  | ARG  |
| 46  | BN    | 41  | ASP  |
| 46  | BN    | 45  | ASN  |
| 46  | BN    | 48  | MET  |
| 46  | BN    | 56  | ASN  |
| 46  | BN    | 63  | THR  |
| 46  | BN    | 65  | LYS  |
| 46  | BN    | 96  | GLU  |
| 46  | BN    | 109 | LYS  |
| 46  | BN    | 123 | TYR  |
| 47  | BO    | 23  | ARG  |
| 47  | BO    | 38  | VAL  |
| 47  | BO    | 40  | VAL  |
| 47  | BO    | 48  | PRO  |
| 47  | BO    | 49  | ARG  |
| 47  | BO    | 80  | ASP  |
| 47  | BO    | 87  | ILE  |
| 47  | BO    | 117 | LEU  |
| 48  | BP    | 7   | ARG  |
| 48  | BP    | 13  | ASN  |
| 48  | BP    | 16  | ARG  |
| 48  | BP    | 18  | ARG  |
| 48  | BP    | 39  | LYS  |
| 48  | BP    | 41  | ARG  |
| 48  | BP    | 42  | SER  |
| 48  | BP    | 51  | PHE  |
| 48  | BP    | 57  | THR  |
| 48  | BP    | 60  | MET  |
| 48  | BP    | 61  | ARG  |
| 48  | BP    | 62  | LEU  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | BP    | 64  | LYS  |
| 48  | BP    | 70  | GLN  |
| 48  | BP    | 81  | GLN  |
| 48  | BP    | 85  | LEU  |
| 48  | BP    | 91  | PHE  |
| 48  | BP    | 108 | LYS  |
| 48  | BP    | 114 | ILE  |
| 48  | BP    | 123 | LEU  |
| 48  | BP    | 149 | GLU  |
| 49  | BQ    | 14  | ARG  |
| 49  | BQ    | 17  | LEU  |
| 49  | BQ    | 45  | GLN  |
| 49  | BQ    | 46  | GLN  |
| 49  | BQ    | 55  | VAL  |
| 49  | BQ    | 56  | ARG  |
| 49  | BQ    | 58  | PHE  |
| 49  | BQ    | 65  | PHE  |
| 49  | BQ    | 67  | ARG  |
| 49  | BQ    | 76  | LYS  |
| 49  | BQ    | 79  | LEU  |
| 49  | BQ    | 81  | VAL  |
| 49  | BQ    | 106 | VAL  |
| 49  | BQ    | 134 | ARG  |
| 49  | BQ    | 135 | ASP  |
| 49  | BQ    | 139 | GLU  |
| 50  | BR    | 8   | ARG  |
| 50  | BR    | 27  | SER  |
| 50  | BR    | 30  | THR  |
| 50  | BR    | 33  | ARG  |
| 50  | BR    | 54  | LEU  |
| 50  | BR    | 71  | GLN  |
| 50  | BR    | 75  | LEU  |
| 50  | BR    | 94  | TYR  |
| 50  | BR    | 97  | VAL  |
| 50  | BR    | 99  | LYS  |
| 50  | BR    | 100 | LEU  |
| 51  | BS    | 11  | LYS  |
| 51  | BS    | 12  | PHE  |
| 51  | BS    | 36  | TYR  |
| 51  | BS    | 63  | THR  |
| 51  | BS    | 67  | ARG  |
| 51  | BS    | 92  | TYR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | BS    | 97  | ARG  |
| 51  | BS    | 101 | LEU  |
| 51  | BS    | 106 | ARG  |
| 52  | BT    | 6   | LEU  |
| 52  | BT    | 13  | ARG  |
| 52  | BT    | 16  | ARG  |
| 52  | BT    | 24  | PRO  |
| 52  | BT    | 32  | TYR  |
| 52  | BT    | 38  | ASN  |
| 52  | BT    | 49  | VAL  |
| 52  | BT    | 53  | ARG  |
| 52  | BT    | 58  | ASN  |
| 52  | BT    | 62  | THR  |
| 52  | BT    | 65  | LYS  |
| 52  | BT    | 78  | LEU  |
| 52  | BT    | 82  | LEU  |
| 52  | BT    | 90  | GLN  |
| 52  | BT    | 93  | ARG  |
| 52  | BT    | 96  | ARG  |
| 52  | BT    | 108 | ARG  |
| 52  | BT    | 115 | ARG  |
| 52  | BT    | 124 | ASP  |
| 52  | BT    | 125 | ARG  |
| 52  | BT    | 128 | GLU  |
| 52  | BT    | 129 | ARG  |
| 52  | BT    | 132 | LYS  |
| 53  | BU    | 20  | LEU  |
| 53  | BU    | 49  | HIS  |
| 53  | BU    | 74  | LEU  |
| 53  | BU    | 76  | TYR  |
| 53  | BU    | 79  | PHE  |
| 53  | BU    | 92  | ARG  |
| 53  | BU    | 101 | ARG  |
| 53  | BU    | 108 | GLU  |
| 53  | BU    | 112 | ARG  |
| 54  | BV    | 1   | MET  |
| 54  | BV    | 18  | LEU  |
| 54  | BV    | 19  | LYS  |
| 54  | BV    | 21  | ARG  |
| 54  | BV    | 39  | LEU  |
| 54  | BV    | 40  | LEU  |
| 54  | BV    | 82  | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | BV    | 89  | GLN  |
| 54  | BV    | 95  | LEU  |
| 54  | BV    | 98  | GLU  |
| 54  | BV    | 99  | ILE  |
| 55  | BW    | 11  | ARG  |
| 55  | BW    | 40  | ASN  |
| 55  | BW    | 52  | GLU  |
| 55  | BW    | 75  | TYR  |
| 55  | BW    | 88  | ARG  |
| 55  | BW    | 98  | LYS  |
| 55  | BW    | 107 | LEU  |
| 56  | BX    | 3   | THR  |
| 56  | BX    | 11  | PRO  |
| 56  | BX    | 27  | THR  |
| 56  | BX    | 28  | PHE  |
| 56  | BX    | 51  | VAL  |
| 56  | BX    | 56  | THR  |
| 56  | BX    | 57  | LEU  |
| 56  | BX    | 68  | ARG  |
| 56  | BX    | 75  | ASP  |
| 56  | BX    | 76  | ARG  |
| 57  | BY    | 2   | ARG  |
| 57  | BY    | 7   | VAL  |
| 57  | BY    | 9   | LYS  |
| 57  | BY    | 29  | GLU  |
| 57  | BY    | 32  | PRO  |
| 57  | BY    | 51  | VAL  |
| 57  | BY    | 53  | PRO  |
| 57  | BY    | 55  | TYR  |
| 57  | BY    | 77  | PRO  |
| 57  | BY    | 79  | CYS  |
| 57  | BY    | 90  | LEU  |
| 57  | BY    | 102 | CYS  |
| 58  | BZ    | 5   | LEU  |
| 58  | BZ    | 6   | LYS  |
| 58  | BZ    | 8   | TYR  |
| 58  | BZ    | 28  | MET  |
| 58  | BZ    | 30  | ASN  |
| 58  | BZ    | 31  | ARG  |
| 58  | BZ    | 34  | ASN  |
| 58  | BZ    | 55  | HIS  |
| 58  | BZ    | 63  | ASP  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 58  | BZ    | 68  | PRO  |
| 58  | BZ    | 72  | ARG  |
| 58  | BZ    | 78  | LYS  |
| 58  | BZ    | 83  | PRO  |
| 58  | BZ    | 87  | ASP  |
| 58  | BZ    | 92  | SER  |
| 58  | BZ    | 107 | THR  |
| 58  | BZ    | 112 | ARG  |
| 58  | BZ    | 123 | ASP  |
| 58  | BZ    | 127 | LYS  |
| 58  | BZ    | 140 | ASP  |
| 58  | BZ    | 146 | ILE  |
| 58  | BZ    | 150 | LEU  |
| 58  | BZ    | 154 | ASP  |
| 58  | BZ    | 158 | PRO  |
| 58  | BZ    | 163 | LEU  |
| 58  | BZ    | 166 | SER  |
| 58  | BZ    | 171 | ILE  |
| 58  | BZ    | 186 | GLU  |
| 2   | CB    | 15  | VAL  |
| 2   | CB    | 16  | HIS  |
| 2   | CB    | 17  | PHE  |
| 2   | CB    | 24  | TRP  |
| 2   | CB    | 36  | ARG  |
| 2   | CB    | 43  | ASP  |
| 2   | CB    | 44  | LEU  |
| 2   | CB    | 67  | THR  |
| 2   | CB    | 79  | ASP  |
| 2   | CB    | 101 | MET  |
| 2   | CB    | 111 | ARG  |
| 2   | CB    | 129 | GLU  |
| 2   | CB    | 137 | ARG  |
| 2   | CB    | 157 | ARG  |
| 2   | CB    | 162 | ILE  |
| 2   | CB    | 172 | ILE  |
| 2   | CB    | 178 | ARG  |
| 2   | CB    | 192 | SER  |
| 2   | CB    | 200 | ILE  |
| 2   | CB    | 204 | ASN  |
| 2   | CB    | 212 | GLN  |
| 2   | CB    | 220 | ASP  |
| 2   | CB    | 221 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CC    | 5   | ILE  |
| 3   | CC    | 16  | ARG  |
| 3   | CC    | 29  | TYR  |
| 3   | CC    | 34  | LEU  |
| 3   | CC    | 56  | ASP  |
| 3   | CC    | 72  | LYS  |
| 3   | CC    | 79  | ARG  |
| 3   | CC    | 85  | ARG  |
| 3   | CC    | 95  | THR  |
| 3   | CC    | 98  | ASN  |
| 3   | CC    | 125 | GLU  |
| 3   | CC    | 127 | ARG  |
| 3   | CC    | 152 | ILE  |
| 3   | CC    | 156 | ARG  |
| 3   | CC    | 165 | THR  |
| 3   | CC    | 167 | TRP  |
| 3   | CC    | 178 | LEU  |
| 3   | CC    | 179 | ARG  |
| 4   | CD    | 3   | ARG  |
| 4   | CD    | 9   | CYS  |
| 4   | CD    | 12  | CYS  |
| 4   | CD    | 15  | GLU  |
| 4   | CD    | 22  | LYS  |
| 4   | CD    | 36  | ARG  |
| 4   | CD    | 49  | ARG  |
| 4   | CD    | 53  | ASP  |
| 4   | CD    | 57  | ARG  |
| 4   | CD    | 70  | ILE  |
| 4   | CD    | 73  | ARG  |
| 4   | CD    | 78  | LEU  |
| 4   | CD    | 96  | LEU  |
| 4   | CD    | 114 | ARG  |
| 4   | CD    | 127 | THR  |
| 4   | CD    | 131 | ARG  |
| 4   | CD    | 132 | ARG  |
| 4   | CD    | 135 | LEU  |
| 4   | CD    | 162 | LEU  |
| 4   | CD    | 168 | ARG  |
| 5   | CE    | 12  | LEU  |
| 5   | CE    | 18  | ARG  |
| 5   | CE    | 20  | GLN  |
| 5   | CE    | 31  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | CE    | 41  | VAL  |
| 5   | CE    | 47  | LYS  |
| 5   | CE    | 56  | GLN  |
| 5   | CE    | 64  | ARG  |
| 5   | CE    | 72  | GLN  |
| 5   | CE    | 75  | THR  |
| 5   | CE    | 76  | ILE  |
| 5   | CE    | 79  | GLU  |
| 5   | CE    | 101 | ILE  |
| 5   | CE    | 117 | ASP  |
| 5   | CE    | 144 | THR  |
| 6   | CF    | 15  | ASP  |
| 6   | CF    | 32  | ASN  |
| 6   | CF    | 43  | LEU  |
| 6   | CF    | 47  | ARG  |
| 6   | CF    | 69  | GLU  |
| 6   | CF    | 86  | ARG  |
| 6   | CF    | 98  | LEU  |
| 7   | CG    | 27  | ILE  |
| 7   | CG    | 57  | GLU  |
| 7   | CG    | 66  | VAL  |
| 7   | CG    | 79  | ARG  |
| 7   | CG    | 104 | LEU  |
| 7   | CG    | 113 | GLU  |
| 7   | CG    | 124 | LEU  |
| 7   | CG    | 137 | LYS  |
| 7   | CG    | 151 | TYR  |
| 8   | CH    | 1   | MET  |
| 8   | CH    | 25  | ASP  |
| 8   | CH    | 54  | ASP  |
| 8   | CH    | 91  | ARG  |
| 8   | CH    | 98  | LYS  |
| 8   | CH    | 102 | ARG  |
| 8   | CH    | 118 | VAL  |
| 9   | CI    | 4   | TYR  |
| 9   | CI    | 10  | ARG  |
| 9   | CI    | 29  | ASN  |
| 9   | CI    | 59  | PHE  |
| 9   | CI    | 95  | LYS  |
| 9   | CI    | 114 | TYR  |
| 9   | CI    | 121 | ARG  |
| 9   | CI    | 128 | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | CJ    | 22  | LYS  |
| 10  | CJ    | 40  | LEU  |
| 10  | CJ    | 43  | ARG  |
| 10  | CJ    | 50  | ILE  |
| 10  | CJ    | 55  | LYS  |
| 10  | CJ    | 59  | SER  |
| 10  | CJ    | 62  | HIS  |
| 10  | CJ    | 63  | PHE  |
| 10  | CJ    | 74  | ILE  |
| 10  | CJ    | 76  | ASN  |
| 10  | CJ    | 96  | ILE  |
| 11  | CK    | 29  | ILE  |
| 11  | CK    | 87  | THR  |
| 11  | CK    | 91  | ARG  |
| 11  | CK    | 92  | GLU  |
| 11  | CK    | 117 | ASN  |
| 11  | CK    | 124 | LYS  |
| 12  | CL    | 7   | ILE  |
| 12  | CL    | 20  | LYS  |
| 12  | CL    | 38  | THR  |
| 12  | CL    | 41  | ARG  |
| 12  | CL    | 47  | LYS  |
| 12  | CL    | 53  | ARG  |
| 12  | CL    | 70  | ILE  |
| 12  | CL    | 81  | SER  |
| 12  | CL    | 85  | ILE  |
| 12  | CL    | 98  | TYR  |
| 12  | CL    | 113 | ARG  |
| 13  | CM    | 64  | TRP  |
| 13  | CM    | 66  | LEU  |
| 13  | CM    | 108 | ARG  |
| 13  | CM    | 113 | PRO  |
| 13  | CM    | 115 | LYS  |
| 13  | CM    | 120 | LYS  |
| 13  | CM    | 121 | LYS  |
| 13  | CM    | 124 | PRO  |
| 14  | CN    | 14  | PRO  |
| 14  | CN    | 16  | PHE  |
| 14  | CN    | 29  | ARG  |
| 14  | CN    | 41  | ARG  |
| 14  | CN    | 42  | ILE  |
| 14  | CN    | 44  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | CO    | 10  | LYS  |
| 15  | CO    | 39  | LEU  |
| 15  | CO    | 41  | GLU  |
| 15  | CO    | 57  | LEU  |
| 15  | CO    | 65  | ARG  |
| 15  | CO    | 82  | ILE  |
| 15  | CO    | 85  | LEU  |
| 15  | CO    | 88  | ARG  |
| 16  | CP    | 1   | MET  |
| 16  | CP    | 2   | VAL  |
| 16  | CP    | 6   | LEU  |
| 16  | CP    | 11  | SER  |
| 16  | CP    | 32  | TYR  |
| 17  | CQ    | 7   | THR  |
| 17  | CQ    | 9   | VAL  |
| 17  | CQ    | 23  | VAL  |
| 17  | CQ    | 35  | VAL  |
| 17  | CQ    | 48  | GLU  |
| 17  | CQ    | 52  | LYS  |
| 17  | CQ    | 78  | GLU  |
| 18  | CR    | 29  | PHE  |
| 18  | CR    | 31  | LEU  |
| 19  | CS    | 5   | LEU  |
| 19  | CS    | 6   | LYS  |
| 19  | CS    | 7   | LYS  |
| 19  | CS    | 15  | LEU  |
| 19  | CS    | 19  | VAL  |
| 19  | CS    | 29  | ARG  |
| 19  | CS    | 37  | ARG  |
| 19  | CS    | 44  | MET  |
| 19  | CS    | 66  | MET  |
| 19  | CS    | 77  | THR  |
| 20  | CT    | 13  | LEU  |
| 20  | CT    | 24  | LEU  |
| 20  | CT    | 26  | ASN  |
| 20  | CT    | 36  | LEU  |
| 20  | CT    | 74  | LYS  |
| 20  | CT    | 84  | LEU  |
| 20  | CT    | 93  | GLU  |
| 24  | CY    | 6   | GLU  |
| 24  | CY    | 13  | ARG  |
| 24  | CY    | 14  | ASN  |

*Continued on next page...*



*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 24         | CY           | 21         | ILE         |
| 24         | CY           | 34         | TYR         |
| 24         | CY           | 65         | ILE         |
| 24         | CY           | 66         | THR         |
| 24         | CY           | 79         | ILE         |
| 24         | CY           | 81         | ILE         |
| 24         | CY           | 88         | VAL         |
| 24         | CY           | 90         | PHE         |
| 24         | CY           | 92         | ILE         |
| 24         | CY           | 95         | GLU         |
| 24         | CY           | 100        | VAL         |
| 24         | CY           | 101        | LEU         |
| 24         | CY           | 102        | ASP         |
| 24         | CY           | 117        | GLN         |
| 24         | CY           | 128        | TYR         |
| 24         | CY           | 130        | VAL         |
| 24         | CY           | 132        | ARG         |
| 24         | CY           | 137        | ASN         |
| 24         | CY           | 157        | LEU         |
| 24         | CY           | 175        | SER         |
| 24         | CY           | 191        | ASP         |
| 24         | CY           | 192        | LEU         |
| 24         | CY           | 216        | LEU         |
| 24         | CY           | 225        | GLU         |
| 24         | CY           | 232        | LEU         |
| 24         | CY           | 255        | ILE         |
| 24         | CY           | 260        | LEU         |
| 24         | CY           | 278        | ASP         |
| 24         | CY           | 312        | LEU         |
| 24         | CY           | 326        | THR         |
| 24         | CY           | 343        | ASN         |
| 24         | CY           | 357        | ARG         |
| 24         | CY           | 381        | LYS         |
| 24         | CY           | 388        | THR         |
| 24         | CY           | 396        | ARG         |
| 24         | CY           | 397        | VAL         |
| 24         | CY           | 399        | LEU         |
| 24         | CY           | 415        | PRO         |
| 24         | CY           | 420        | ASP         |
| 24         | CY           | 421        | GLN         |
| 24         | CY           | 422        | GLU         |
| 24         | CY           | 428        | LEU         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | CY    | 438 | PHE  |
| 24  | CY    | 459 | LEU  |
| 24  | CY    | 476 | VAL  |
| 24  | CY    | 487 | ILE  |
| 24  | CY    | 492 | ASP  |
| 24  | CY    | 499 | ARG  |
| 24  | CY    | 504 | ARG  |
| 24  | CY    | 507 | TYR  |
| 24  | CY    | 512 | ILE  |
| 24  | CY    | 527 | ASN  |
| 24  | CY    | 548 | GLU  |
| 24  | CY    | 572 | TYR  |
| 24  | CY    | 575 | VAL  |
| 24  | CY    | 580 | MET  |
| 24  | CY    | 598 | ASP  |
| 24  | CY    | 614 | GLU  |
| 24  | CY    | 634 | MET  |
| 24  | CY    | 641 | GLN  |
| 24  | CY    | 644 | ARG  |
| 24  | CY    | 647 | VAL  |
| 24  | CY    | 661 | SER  |
| 24  | CY    | 674 | ASP  |
| 24  | CY    | 683 | VAL  |
| 25  | D0    | 5   | LYS  |
| 25  | D0    | 11  | ARG  |
| 25  | D0    | 20  | ARG  |
| 25  | D0    | 27  | GLU  |
| 25  | D0    | 41  | ARG  |
| 25  | D0    | 60  | PHE  |
| 25  | D0    | 75  | LEU  |
| 25  | D0    | 78  | TYR  |
| 25  | D0    | 84  | LEU  |
| 26  | D1    | 20  | ARG  |
| 26  | D1    | 39  | LYS  |
| 26  | D1    | 45  | ASN  |
| 26  | D1    | 46  | LEU  |
| 26  | D1    | 50  | ARG  |
| 26  | D1    | 61  | ARG  |
| 26  | D1    | 80  | LEU  |
| 26  | D1    | 83  | GLU  |
| 27  | D2    | 20  | GLU  |
| 27  | D2    | 37  | PHE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | D2    | 53  | LEU  |
| 27  | D2    | 56  | GLN  |
| 27  | D2    | 57  | ILE  |
| 27  | D2    | 59  | ARG  |
| 27  | D2    | 60  | LEU  |
| 27  | D2    | 63  | VAL  |
| 28  | D3    | 8   | LEU  |
| 28  | D3    | 28  | LEU  |
| 28  | D3    | 38  | GLU  |
| 28  | D3    | 48  | GLU  |
| 29  | D4    | 1   | MET  |
| 29  | D4    | 5   | ILE  |
| 29  | D4    | 8   | LYS  |
| 29  | D4    | 9   | LEU  |
| 29  | D4    | 13  | ARG  |
| 29  | D4    | 20  | ASN  |
| 29  | D4    | 32  | TYR  |
| 29  | D4    | 39  | CYS  |
| 29  | D4    | 40  | HIS  |
| 29  | D4    | 42  | PHE  |
| 29  | D4    | 43  | TYR  |
| 29  | D4    | 49  | PHE  |
| 29  | D4    | 51  | ASP  |
| 29  | D4    | 55  | ARG  |
| 30  | D5    | 3   | LYS  |
| 30  | D5    | 4   | HIS  |
| 30  | D5    | 23  | HIS  |
| 30  | D5    | 36  | CYS  |
| 30  | D5    | 55  | ARG  |
| 30  | D5    | 58  | LEU  |
| 31  | D6    | 6   | ARG  |
| 31  | D6    | 9   | LEU  |
| 31  | D6    | 10  | LEU  |
| 31  | D6    | 11  | LEU  |
| 31  | D6    | 15  | GLU  |
| 31  | D6    | 23  | THR  |
| 31  | D6    | 28  | ARG  |
| 31  | D6    | 30  | THR  |
| 31  | D6    | 31  | PRO  |
| 31  | D6    | 39  | TYR  |
| 31  | D6    | 42  | TRP  |
| 32  | D7    | 1   | MET  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | D7    | 4   | THR  |
| 32  | D7    | 8   | ASN  |
| 32  | D7    | 41  | ARG  |
| 32  | D7    | 48  | LYS  |
| 33  | D8    | 6   | THR  |
| 33  | D8    | 30  | ARG  |
| 33  | D8    | 32  | LEU  |
| 33  | D8    | 33  | ASN  |
| 33  | D8    | 34  | TRP  |
| 33  | D8    | 44  | LYS  |
| 33  | D8    | 48  | PHE  |
| 33  | D8    | 49  | VAL  |
| 33  | D8    | 61  | LEU  |
| 33  | D8    | 64  | TYR  |
| 34  | D9    | 1   | MET  |
| 34  | D9    | 2   | LYS  |
| 34  | D9    | 10  | ILE  |
| 34  | D9    | 11  | CYS  |
| 34  | D9    | 29  | ASN  |
| 37  | DC    | 18  | ASN  |
| 37  | DC    | 53  | ARG  |
| 37  | DC    | 54  | ARG  |
| 37  | DC    | 74  | ARG  |
| 37  | DC    | 121 | MET  |
| 37  | DC    | 149 | ASN  |
| 37  | DC    | 184 | GLU  |
| 37  | DC    | 185 | LYS  |
| 37  | DC    | 189 | ASN  |
| 37  | DC    | 191 | ARG  |
| 37  | DC    | 212 | SER  |
| 38  | DD    | 10  | THR  |
| 38  | DD    | 23  | GLU  |
| 38  | DD    | 24  | ILE  |
| 38  | DD    | 26  | LYS  |
| 38  | DD    | 35  | LYS  |
| 38  | DD    | 37  | LEU  |
| 38  | DD    | 43  | ARG  |
| 38  | DD    | 61  | LEU  |
| 38  | DD    | 63  | ARG  |
| 38  | DD    | 65  | ILE  |
| 38  | DD    | 87  | ASN  |
| 38  | DD    | 89  | SER  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | DD    | 92  | ILE  |
| 38  | DD    | 94  | LEU  |
| 38  | DD    | 95  | LEU  |
| 38  | DD    | 96  | HIS  |
| 38  | DD    | 104 | TYR  |
| 38  | DD    | 106 | ILE  |
| 38  | DD    | 111 | LEU  |
| 38  | DD    | 117 | VAL  |
| 38  | DD    | 131 | LEU  |
| 38  | DD    | 157 | ARG  |
| 38  | DD    | 166 | GLN  |
| 38  | DD    | 183 | ARG  |
| 38  | DD    | 190 | TYR  |
| 38  | DD    | 192 | THR  |
| 38  | DD    | 202 | LYS  |
| 38  | DD    | 212 | SER  |
| 38  | DD    | 221 | VAL  |
| 38  | DD    | 227 | ASN  |
| 38  | DD    | 228 | PRO  |
| 38  | DD    | 244 | ARG  |
| 38  | DD    | 246 | PRO  |
| 38  | DD    | 257 | LEU  |
| 38  | DD    | 260 | ARG  |
| 38  | DD    | 270 | ILE  |
| 38  | DD    | 271 | ILE  |
| 38  | DD    | 273 | ARG  |
| 38  | DD    | 275 | LYS  |
| 39  | DE    | 4   | ILE  |
| 39  | DE    | 9   | VAL  |
| 39  | DE    | 18  | ASP  |
| 39  | DE    | 36  | ARG  |
| 39  | DE    | 49  | LEU  |
| 39  | DE    | 55  | ASN  |
| 39  | DE    | 61  | ARG  |
| 39  | DE    | 67  | PHE  |
| 39  | DE    | 69  | LYS  |
| 39  | DE    | 78  | LEU  |
| 39  | DE    | 79  | ARG  |
| 39  | DE    | 94  | GLU  |
| 39  | DE    | 95  | ILE  |
| 39  | DE    | 113 | PHE  |
| 39  | DE    | 118 | LYS  |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 39         | DE           | 119        | ARG         |
| 39         | DE           | 121        | ASN         |
| 39         | DE           | 134        | ILE         |
| 39         | DE           | 144        | ARG         |
| 39         | DE           | 178        | GLU         |
| 39         | DE           | 184        | VAL         |
| 39         | DE           | 192        | ASN         |
| 39         | DE           | 197        | ILE         |
| 39         | DE           | 202        | LYS         |
| 39         | DE           | 203        | LYS         |
| 40         | DF           | 19         | GLU         |
| 40         | DF           | 28         | ILE         |
| 40         | DF           | 41         | LEU         |
| 40         | DF           | 64         | ILE         |
| 40         | DF           | 66         | PRO         |
| 40         | DF           | 83         | PHE         |
| 40         | DF           | 125        | LEU         |
| 40         | DF           | 149        | ASP         |
| 40         | DF           | 160        | ASN         |
| 40         | DF           | 165        | ARG         |
| 40         | DF           | 175        | THR         |
| 40         | DF           | 179        | GLU         |
| 41         | DG           | 4          | ASP         |
| 41         | DG           | 22         | ARG         |
| 41         | DG           | 26         | GLN         |
| 41         | DG           | 33         | ARG         |
| 41         | DG           | 34         | LEU         |
| 41         | DG           | 37         | VAL         |
| 41         | DG           | 38         | VAL         |
| 41         | DG           | 40         | ASN         |
| 41         | DG           | 43         | LEU         |
| 41         | DG           | 45         | GLU         |
| 41         | DG           | 47         | LYS         |
| 41         | DG           | 49         | ASP         |
| 41         | DG           | 51         | ARG         |
| 41         | DG           | 62         | LEU         |
| 41         | DG           | 67         | LYS         |
| 41         | DG           | 80         | PHE         |
| 41         | DG           | 82         | LEU         |
| 41         | DG           | 83         | ARG         |
| 41         | DG           | 98         | ARG         |
| 41         | DG           | 118        | ARG         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41  | DG    | 120 | LEU  |
| 41  | DG    | 123 | ASN  |
| 41  | DG    | 135 | LEU  |
| 41  | DG    | 143 | GLU  |
| 41  | DG    | 145 | THR  |
| 41  | DG    | 148 | MET  |
| 41  | DG    | 159 | VAL  |
| 41  | DG    | 166 | ASP  |
| 41  | DG    | 167 | GLU  |
| 42  | DH    | 46  | GLU  |
| 42  | DH    | 49  | VAL  |
| 42  | DH    | 53  | GLU  |
| 42  | DH    | 54  | ARG  |
| 42  | DH    | 83  | TYR  |
| 42  | DH    | 89  | ILE  |
| 42  | DH    | 104 | GLU  |
| 42  | DH    | 105 | LEU  |
| 42  | DH    | 143 | GLN  |
| 42  | DH    | 158 | HIS  |
| 44  | DK    | 2   | LYS  |
| 44  | DK    | 3   | LYS  |
| 44  | DK    | 29  | GLN  |
| 44  | DK    | 30  | HIS  |
| 44  | DK    | 34  | ILE  |
| 44  | DK    | 38  | VAL  |
| 44  | DK    | 47  | ASN  |
| 44  | DK    | 65  | PHE  |
| 44  | DK    | 70  | LYS  |
| 44  | DK    | 77  | LEU  |
| 44  | DK    | 86  | LYS  |
| 44  | DK    | 95  | LYS  |
| 44  | DK    | 105 | LEU  |
| 44  | DK    | 117 | THR  |
| 46  | DN    | 1   | MET  |
| 46  | DN    | 4   | TYR  |
| 46  | DN    | 23  | LEU  |
| 46  | DN    | 26  | LEU  |
| 46  | DN    | 39  | ARG  |
| 46  | DN    | 41  | ASP  |
| 46  | DN    | 45  | ASN  |
| 46  | DN    | 48  | MET  |
| 46  | DN    | 56  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | DN    | 63  | THR  |
| 46  | DN    | 65  | LYS  |
| 46  | DN    | 78  | TYR  |
| 46  | DN    | 96  | GLU  |
| 46  | DN    | 109 | LYS  |
| 46  | DN    | 123 | TYR  |
| 47  | DO    | 23  | ARG  |
| 47  | DO    | 38  | VAL  |
| 47  | DO    | 40  | VAL  |
| 47  | DO    | 48  | PRO  |
| 47  | DO    | 49  | ARG  |
| 47  | DO    | 80  | ASP  |
| 47  | DO    | 87  | ILE  |
| 47  | DO    | 117 | LEU  |
| 48  | DP    | 7   | ARG  |
| 48  | DP    | 13  | ASN  |
| 48  | DP    | 16  | ARG  |
| 48  | DP    | 18  | ARG  |
| 48  | DP    | 39  | LYS  |
| 48  | DP    | 41  | ARG  |
| 48  | DP    | 42  | SER  |
| 48  | DP    | 51  | PHE  |
| 48  | DP    | 57  | THR  |
| 48  | DP    | 60  | MET  |
| 48  | DP    | 61  | ARG  |
| 48  | DP    | 62  | LEU  |
| 48  | DP    | 64  | LYS  |
| 48  | DP    | 70  | GLN  |
| 48  | DP    | 81  | GLN  |
| 48  | DP    | 85  | LEU  |
| 48  | DP    | 91  | PHE  |
| 48  | DP    | 108 | LYS  |
| 48  | DP    | 114 | ILE  |
| 48  | DP    | 123 | LEU  |
| 48  | DP    | 149 | GLU  |
| 49  | DQ    | 14  | ARG  |
| 49  | DQ    | 45  | GLN  |
| 49  | DQ    | 46  | GLN  |
| 49  | DQ    | 55  | VAL  |
| 49  | DQ    | 56  | ARG  |
| 49  | DQ    | 58  | PHE  |
| 49  | DQ    | 65  | PHE  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49  | DQ    | 67  | ARG  |
| 49  | DQ    | 76  | LYS  |
| 49  | DQ    | 79  | LEU  |
| 49  | DQ    | 81  | VAL  |
| 49  | DQ    | 134 | ARG  |
| 49  | DQ    | 135 | ASP  |
| 49  | DQ    | 139 | GLU  |
| 50  | DR    | 8   | ARG  |
| 50  | DR    | 27  | SER  |
| 50  | DR    | 30  | THR  |
| 50  | DR    | 33  | ARG  |
| 50  | DR    | 54  | LEU  |
| 50  | DR    | 65  | LEU  |
| 50  | DR    | 71  | GLN  |
| 50  | DR    | 75  | LEU  |
| 50  | DR    | 94  | TYR  |
| 50  | DR    | 97  | VAL  |
| 50  | DR    | 99  | LYS  |
| 50  | DR    | 100 | LEU  |
| 51  | DS    | 11  | LYS  |
| 51  | DS    | 12  | PHE  |
| 51  | DS    | 36  | TYR  |
| 51  | DS    | 63  | THR  |
| 51  | DS    | 67  | ARG  |
| 51  | DS    | 92  | TYR  |
| 51  | DS    | 97  | ARG  |
| 51  | DS    | 101 | LEU  |
| 51  | DS    | 106 | ARG  |
| 52  | DT    | 6   | LEU  |
| 52  | DT    | 13  | ARG  |
| 52  | DT    | 16  | ARG  |
| 52  | DT    | 24  | PRO  |
| 52  | DT    | 32  | TYR  |
| 52  | DT    | 38  | ASN  |
| 52  | DT    | 49  | VAL  |
| 52  | DT    | 53  | ARG  |
| 52  | DT    | 58  | ASN  |
| 52  | DT    | 62  | THR  |
| 52  | DT    | 65  | LYS  |
| 52  | DT    | 78  | LEU  |
| 52  | DT    | 82  | LEU  |
| 52  | DT    | 90  | GLN  |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 52         | DT           | 93         | ARG         |
| 52         | DT           | 96         | ARG         |
| 52         | DT           | 108        | ARG         |
| 52         | DT           | 115        | ARG         |
| 52         | DT           | 124        | ASP         |
| 52         | DT           | 125        | ARG         |
| 52         | DT           | 128        | GLU         |
| 52         | DT           | 129        | ARG         |
| 52         | DT           | 132        | LYS         |
| 53         | DU           | 20         | LEU         |
| 53         | DU           | 49         | HIS         |
| 53         | DU           | 74         | LEU         |
| 53         | DU           | 76         | TYR         |
| 53         | DU           | 79         | PHE         |
| 53         | DU           | 92         | ARG         |
| 53         | DU           | 101        | ARG         |
| 53         | DU           | 108        | GLU         |
| 53         | DU           | 112        | ARG         |
| 54         | DV           | 1          | MET         |
| 54         | DV           | 18         | LEU         |
| 54         | DV           | 19         | LYS         |
| 54         | DV           | 21         | ARG         |
| 54         | DV           | 39         | LEU         |
| 54         | DV           | 40         | LEU         |
| 54         | DV           | 82         | ARG         |
| 54         | DV           | 89         | GLN         |
| 54         | DV           | 95         | LEU         |
| 54         | DV           | 98         | GLU         |
| 54         | DV           | 99         | ILE         |
| 55         | DW           | 11         | ARG         |
| 55         | DW           | 40         | ASN         |
| 55         | DW           | 52         | GLU         |
| 55         | DW           | 75         | TYR         |
| 55         | DW           | 88         | ARG         |
| 55         | DW           | 98         | LYS         |
| 55         | DW           | 107        | LEU         |
| 56         | DX           | 3          | THR         |
| 56         | DX           | 11         | PRO         |
| 56         | DX           | 27         | THR         |
| 56         | DX           | 28         | PHE         |
| 56         | DX           | 51         | VAL         |
| 56         | DX           | 56         | THR         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 56  | DX    | 57  | LEU  |
| 56  | DX    | 68  | ARG  |
| 56  | DX    | 75  | ASP  |
| 56  | DX    | 76  | ARG  |
| 57  | DY    | 2   | ARG  |
| 57  | DY    | 7   | VAL  |
| 57  | DY    | 9   | LYS  |
| 57  | DY    | 29  | GLU  |
| 57  | DY    | 32  | PRO  |
| 57  | DY    | 51  | VAL  |
| 57  | DY    | 53  | PRO  |
| 57  | DY    | 55  | TYR  |
| 57  | DY    | 77  | PRO  |
| 57  | DY    | 79  | CYS  |
| 57  | DY    | 90  | LEU  |
| 57  | DY    | 102 | CYS  |
| 58  | DZ    | 5   | LEU  |
| 58  | DZ    | 6   | LYS  |
| 58  | DZ    | 8   | TYR  |
| 58  | DZ    | 20  | ARG  |
| 58  | DZ    | 24  | LEU  |
| 58  | DZ    | 31  | ARG  |
| 58  | DZ    | 72  | ARG  |
| 58  | DZ    | 81  | ARG  |
| 58  | DZ    | 87  | ASP  |
| 58  | DZ    | 92  | SER  |
| 58  | DZ    | 112 | ARG  |
| 58  | DZ    | 123 | ASP  |
| 58  | DZ    | 140 | ASP  |
| 58  | DZ    | 150 | LEU  |
| 58  | DZ    | 154 | ASP  |
| 58  | DZ    | 168 | GLU  |
| 58  | DZ    | 171 | ILE  |
| 58  | DZ    | 179 | ASP  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (348) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 37  | ASN  |
| 2   | AB    | 40  | HIS  |
| 2   | AB    | 78  | GLN  |
| 2   | AB    | 94  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 110 | GLN  |
| 2   | AB    | 113 | HIS  |
| 2   | AB    | 146 | GLN  |
| 2   | AB    | 204 | ASN  |
| 3   | AC    | 28  | GLN  |
| 3   | AC    | 31  | HIS  |
| 3   | AC    | 37  | GLN  |
| 3   | AC    | 108 | ASN  |
| 3   | AC    | 118 | GLN  |
| 3   | AC    | 170 | GLN  |
| 3   | AC    | 176 | HIS  |
| 3   | AC    | 181 | ASN  |
| 4   | AD    | 62  | GLN  |
| 4   | AD    | 74  | GLN  |
| 4   | AD    | 77  | ASN  |
| 4   | AD    | 129 | ASN  |
| 5   | AE    | 20  | GLN  |
| 5   | AE    | 72  | GLN  |
| 5   | AE    | 73  | ASN  |
| 6   | AF    | 16  | GLN  |
| 6   | AF    | 18  | GLN  |
| 6   | AF    | 27  | GLN  |
| 6   | AF    | 32  | ASN  |
| 6   | AF    | 73  | ASN  |
| 6   | AF    | 100 | ASN  |
| 7   | AG    | 13  | GLN  |
| 7   | AG    | 68  | ASN  |
| 7   | AG    | 84  | ASN  |
| 7   | AG    | 96  | GLN  |
| 7   | AG    | 97  | GLN  |
| 7   | AG    | 106 | GLN  |
| 8   | AH    | 82  | HIS  |
| 9   | AI    | 3   | GLN  |
| 9   | AI    | 58  | HIS  |
| 9   | AI    | 124 | GLN  |
| 10  | AJ    | 56  | HIS  |
| 10  | AJ    | 68  | HIS  |
| 10  | AJ    | 76  | ASN  |
| 10  | AJ    | 84  | GLN  |
| 11  | AK    | 22  | HIS  |
| 11  | AK    | 117 | ASN  |
| 12  | AL    | 9   | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | AL    | 49  | ASN  |
| 12  | AL    | 75  | HIS  |
| 12  | AL    | 99  | HIS  |
| 13  | AM    | 40  | ASN  |
| 13  | AM    | 77  | ASN  |
| 14  | AN    | 49  | HIS  |
| 15  | AO    | 9   | GLN  |
| 15  | AO    | 13  | GLN  |
| 15  | AO    | 37  | ASN  |
| 15  | AO    | 62  | GLN  |
| 17  | AQ    | 16  | GLN  |
| 19  | AS    | 14  | HIS  |
| 19  | AS    | 47  | HIS  |
| 20  | AT    | 26  | ASN  |
| 20  | AT    | 42  | GLN  |
| 20  | AT    | 45  | GLN  |
| 20  | AT    | 75  | ASN  |
| 24  | AY    | 14  | ASN  |
| 24  | AY    | 124 | GLN  |
| 24  | AY    | 137 | ASN  |
| 24  | AY    | 165 | GLN  |
| 24  | AY    | 208 | GLN  |
| 24  | AY    | 343 | ASN  |
| 24  | AY    | 421 | GLN  |
| 24  | AY    | 458 | HIS  |
| 24  | AY    | 475 | ASN  |
| 24  | AY    | 500 | GLN  |
| 24  | AY    | 527 | ASN  |
| 24  | AY    | 573 | HIS  |
| 24  | AY    | 630 | GLN  |
| 24  | AY    | 641 | GLN  |
| 25  | B0    | 70  | GLN  |
| 26  | B1    | 45  | ASN  |
| 26  | B1    | 56  | GLN  |
| 27  | B2    | 38  | GLN  |
| 27  | B2    | 47  | ASN  |
| 27  | B2    | 56  | GLN  |
| 28  | B3    | 19  | GLN  |
| 28  | B3    | 46  | ASN  |
| 30  | B5    | 22  | HIS  |
| 30  | B5    | 23  | HIS  |
| 30  | B5    | 43  | HIS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | B6    | 20  | ASN  |
| 31  | B6    | 26  | ASN  |
| 31  | B6    | 32  | ASN  |
| 31  | B6    | 49  | HIS  |
| 32  | B7    | 8   | ASN  |
| 33  | B8    | 31  | HIS  |
| 33  | B8    | 33  | ASN  |
| 33  | B8    | 43  | GLN  |
| 34  | B9    | 29  | ASN  |
| 37  | BC    | 58  | ASN  |
| 37  | BC    | 149 | ASN  |
| 37  | BC    | 166 | ASN  |
| 38  | BD    | 58  | HIS  |
| 38  | BD    | 115 | GLN  |
| 38  | BD    | 116 | GLN  |
| 38  | BD    | 126 | GLN  |
| 38  | BD    | 166 | GLN  |
| 38  | BD    | 186 | HIS  |
| 38  | BD    | 198 | ASN  |
| 38  | BD    | 227 | ASN  |
| 39  | BE    | 48  | GLN  |
| 39  | BE    | 54  | GLN  |
| 39  | BE    | 55  | ASN  |
| 39  | BE    | 129 | HIS  |
| 39  | BE    | 143 | ASN  |
| 39  | BE    | 169 | ASN  |
| 39  | BE    | 192 | ASN  |
| 40  | BF    | 8   | GLN  |
| 40  | BF    | 69  | HIS  |
| 40  | BF    | 75  | HIS  |
| 40  | BF    | 133 | ASN  |
| 40  | BF    | 160 | ASN  |
| 40  | BF    | 169 | ASN  |
| 40  | BF    | 204 | ASN  |
| 41  | BG    | 27  | ASN  |
| 42  | BH    | 65  | HIS  |
| 42  | BH    | 147 | ASN  |
| 42  | BH    | 158 | HIS  |
| 44  | BK    | 29  | GLN  |
| 44  | BK    | 47  | ASN  |
| 44  | BK    | 89  | HIS  |
| 46  | BN    | 45  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 46         | BN           | 56         | ASN         |
| 46         | BN           | 101        | HIS         |
| 46         | BN           | 131        | GLN         |
| 47         | BO           | 5          | GLN         |
| 47         | BO           | 82         | ASN         |
| 48         | BP           | 9          | ASN         |
| 48         | BP           | 13         | ASN         |
| 48         | BP           | 27         | HIS         |
| 48         | BP           | 84         | ASN         |
| 48         | BP           | 128        | HIS         |
| 49         | BQ           | 12         | GLN         |
| 49         | BQ           | 13         | GLN         |
| 49         | BQ           | 45         | GLN         |
| 50         | BR           | 3          | HIS         |
| 50         | BR           | 16         | HIS         |
| 50         | BR           | 23         | ASN         |
| 50         | BR           | 61         | HIS         |
| 52         | BT           | 38         | ASN         |
| 52         | BT           | 43         | GLN         |
| 52         | BT           | 58         | ASN         |
| 52         | BT           | 84         | GLN         |
| 52         | BT           | 90         | GLN         |
| 53         | BU           | 14         | HIS         |
| 53         | BU           | 44         | ASN         |
| 53         | BU           | 49         | HIS         |
| 53         | BU           | 66         | ASN         |
| 53         | BU           | 81         | HIS         |
| 53         | BU           | 94         | ASN         |
| 53         | BU           | 117        | GLN         |
| 54         | BV           | 11         | GLN         |
| 55         | BW           | 61         | ASN         |
| 55         | BW           | 102        | HIS         |
| 56         | BX           | 41         | ASN         |
| 56         | BX           | 55         | ASN         |
| 56         | BX           | 82         | GLN         |
| 58         | BZ           | 54         | HIS         |
| 58         | BZ           | 65         | GLN         |
| 58         | BZ           | 118        | GLN         |
| 58         | BZ           | 121        | HIS         |
| 2          | CB           | 37         | ASN         |
| 2          | CB           | 40         | HIS         |
| 2          | CB           | 78         | GLN         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | CB    | 94  | ASN  |
| 2   | CB    | 110 | GLN  |
| 2   | CB    | 113 | HIS  |
| 2   | CB    | 146 | GLN  |
| 2   | CB    | 204 | ASN  |
| 3   | CC    | 28  | GLN  |
| 3   | CC    | 31  | HIS  |
| 3   | CC    | 37  | GLN  |
| 3   | CC    | 108 | ASN  |
| 3   | CC    | 118 | GLN  |
| 3   | CC    | 170 | GLN  |
| 3   | CC    | 176 | HIS  |
| 3   | CC    | 181 | ASN  |
| 4   | CD    | 62  | GLN  |
| 4   | CD    | 74  | GLN  |
| 4   | CD    | 77  | ASN  |
| 4   | CD    | 129 | ASN  |
| 5   | CE    | 20  | GLN  |
| 5   | CE    | 72  | GLN  |
| 5   | CE    | 73  | ASN  |
| 6   | CF    | 16  | GLN  |
| 6   | CF    | 18  | GLN  |
| 6   | CF    | 27  | GLN  |
| 6   | CF    | 32  | ASN  |
| 6   | CF    | 73  | ASN  |
| 6   | CF    | 100 | ASN  |
| 7   | CG    | 13  | GLN  |
| 7   | CG    | 68  | ASN  |
| 7   | CG    | 84  | ASN  |
| 7   | CG    | 96  | GLN  |
| 7   | CG    | 97  | GLN  |
| 7   | CG    | 106 | GLN  |
| 8   | CH    | 82  | HIS  |
| 9   | CI    | 3   | GLN  |
| 9   | CI    | 58  | HIS  |
| 9   | CI    | 124 | GLN  |
| 10  | CJ    | 56  | HIS  |
| 10  | CJ    | 68  | HIS  |
| 10  | CJ    | 76  | ASN  |
| 10  | CJ    | 84  | GLN  |
| 11  | CK    | 22  | HIS  |
| 11  | CK    | 117 | ASN  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | CL    | 9   | GLN  |
| 12  | CL    | 49  | ASN  |
| 12  | CL    | 75  | HIS  |
| 13  | CM    | 40  | ASN  |
| 13  | CM    | 77  | ASN  |
| 13  | CM    | 101 | GLN  |
| 14  | CN    | 49  | HIS  |
| 15  | CO    | 9   | GLN  |
| 15  | CO    | 13  | GLN  |
| 15  | CO    | 37  | ASN  |
| 15  | CO    | 62  | GLN  |
| 17  | CQ    | 16  | GLN  |
| 19  | CS    | 14  | HIS  |
| 19  | CS    | 47  | HIS  |
| 20  | CT    | 16  | HIS  |
| 20  | CT    | 26  | ASN  |
| 20  | CT    | 42  | GLN  |
| 20  | CT    | 45  | GLN  |
| 20  | CT    | 75  | ASN  |
| 24  | CY    | 40  | HIS  |
| 24  | CY    | 117 | GLN  |
| 24  | CY    | 137 | ASN  |
| 24  | CY    | 165 | GLN  |
| 24  | CY    | 270 | GLN  |
| 24  | CY    | 343 | ASN  |
| 24  | CY    | 421 | GLN  |
| 24  | CY    | 448 | GLN  |
| 24  | CY    | 458 | HIS  |
| 24  | CY    | 480 | GLN  |
| 24  | CY    | 500 | GLN  |
| 24  | CY    | 527 | ASN  |
| 24  | CY    | 543 | GLN  |
| 24  | CY    | 573 | HIS  |
| 24  | CY    | 625 | ASN  |
| 24  | CY    | 630 | GLN  |
| 24  | CY    | 664 | GLN  |
| 25  | D0    | 12  | ASN  |
| 25  | D0    | 70  | GLN  |
| 26  | D1    | 45  | ASN  |
| 26  | D1    | 56  | GLN  |
| 27  | D2    | 38  | GLN  |
| 27  | D2    | 47  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | D2    | 65  | ASN  |
| 28  | D3    | 19  | GLN  |
| 28  | D3    | 46  | ASN  |
| 30  | D5    | 43  | HIS  |
| 31  | D6    | 20  | ASN  |
| 31  | D6    | 26  | ASN  |
| 31  | D6    | 32  | ASN  |
| 31  | D6    | 49  | HIS  |
| 32  | D7    | 8   | ASN  |
| 33  | D8    | 31  | HIS  |
| 33  | D8    | 33  | ASN  |
| 33  | D8    | 43  | GLN  |
| 34  | D9    | 29  | ASN  |
| 37  | DC    | 58  | ASN  |
| 37  | DC    | 149 | ASN  |
| 37  | DC    | 166 | ASN  |
| 38  | DD    | 58  | HIS  |
| 38  | DD    | 96  | HIS  |
| 38  | DD    | 115 | GLN  |
| 38  | DD    | 116 | GLN  |
| 38  | DD    | 126 | GLN  |
| 38  | DD    | 166 | GLN  |
| 38  | DD    | 186 | HIS  |
| 38  | DD    | 198 | ASN  |
| 38  | DD    | 227 | ASN  |
| 38  | DD    | 253 | GLN  |
| 39  | DE    | 48  | GLN  |
| 39  | DE    | 54  | GLN  |
| 39  | DE    | 55  | ASN  |
| 39  | DE    | 129 | HIS  |
| 39  | DE    | 143 | ASN  |
| 39  | DE    | 169 | ASN  |
| 39  | DE    | 192 | ASN  |
| 40  | DF    | 8   | GLN  |
| 40  | DF    | 69  | HIS  |
| 40  | DF    | 75  | HIS  |
| 40  | DF    | 133 | ASN  |
| 40  | DF    | 160 | ASN  |
| 40  | DF    | 169 | ASN  |
| 40  | DF    | 204 | ASN  |
| 41  | DG    | 27  | ASN  |
| 41  | DG    | 41  | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41  | DG    | 58  | GLN  |
| 42  | DH    | 65  | HIS  |
| 42  | DH    | 147 | ASN  |
| 42  | DH    | 158 | HIS  |
| 44  | DK    | 29  | GLN  |
| 44  | DK    | 47  | ASN  |
| 44  | DK    | 89  | HIS  |
| 46  | DN    | 45  | ASN  |
| 46  | DN    | 56  | ASN  |
| 46  | DN    | 101 | HIS  |
| 46  | DN    | 131 | GLN  |
| 47  | DO    | 5   | GLN  |
| 47  | DO    | 82  | ASN  |
| 48  | DP    | 9   | ASN  |
| 48  | DP    | 13  | ASN  |
| 48  | DP    | 27  | HIS  |
| 48  | DP    | 84  | ASN  |
| 48  | DP    | 128 | HIS  |
| 49  | DQ    | 12  | GLN  |
| 49  | DQ    | 13  | GLN  |
| 49  | DQ    | 45  | GLN  |
| 50  | DR    | 3   | HIS  |
| 50  | DR    | 16  | HIS  |
| 50  | DR    | 23  | ASN  |
| 50  | DR    | 61  | HIS  |
| 50  | DR    | 71  | GLN  |
| 51  | DS    | 16  | ASN  |
| 52  | DT    | 38  | ASN  |
| 52  | DT    | 43  | GLN  |
| 52  | DT    | 58  | ASN  |
| 52  | DT    | 84  | GLN  |
| 52  | DT    | 90  | GLN  |
| 53  | DU    | 44  | ASN  |
| 53  | DU    | 49  | HIS  |
| 53  | DU    | 66  | ASN  |
| 53  | DU    | 81  | HIS  |
| 53  | DU    | 94  | ASN  |
| 53  | DU    | 117 | GLN  |
| 54  | DV    | 11  | GLN  |
| 55  | DW    | 61  | ASN  |
| 55  | DW    | 102 | HIS  |
| 56  | DX    | 41  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 56  | DX    | 55  | ASN  |
| 56  | DX    | 82  | GLN  |
| 57  | DY    | 6   | HIS  |
| 58  | DZ    | 54  | HIS  |
| 58  | DZ    | 55  | HIS  |
| 58  | DZ    | 65  | GLN  |
| 58  | DZ    | 73  | GLN  |
| 58  | DZ    | 118 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | AA    | 1503/1522 (98%) | 270 (17%)         | 43 (2%)         |
| 1   | CA    | 1503/1522 (98%) | 266 (17%)         | 43 (2%)         |
| 22  | AV    | 76/77 (98%)     | 15 (19%)          | 0               |
| 22  | AW    | 76/77 (98%)     | 25 (32%)          | 1 (1%)          |
| 22  | CV    | 76/77 (98%)     | 14 (18%)          | 0               |
| 22  | CW    | 76/77 (98%)     | 19 (25%)          | 1 (1%)          |
| 23  | AX    | 11/25 (44%)     | 4 (36%)           | 1 (9%)          |
| 23  | CX    | 11/25 (44%)     | 4 (36%)           | 1 (9%)          |
| 35  | BA    | 2900/2915 (99%) | 597 (20%)         | 71 (2%)         |
| 35  | DA    | 2900/2915 (99%) | 594 (20%)         | 71 (2%)         |
| 36  | BB    | 118/122 (96%)   | 25 (21%)          | 0               |
| 36  | DB    | 118/122 (96%)   | 25 (21%)          | 0               |
| All | All   | 9368/9476 (98%) | 1858 (19%)        | 232 (2%)        |

All (1858) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 9   | G    |
| 1   | AA    | 31  | G    |
| 1   | AA    | 32  | A    |
| 1   | AA    | 33  | A    |
| 1   | AA    | 39  | G    |
| 1   | AA    | 47  | C    |
| 1   | AA    | 48  | C    |
| 1   | AA    | 51  | A    |
| 1   | AA    | 60  | A    |
| 1   | AA    | 61  | G    |
| 1   | AA    | 62  | U    |
| 1   | AA    | 81  | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | AA    | 88     | A    |
| 1   | AA    | 89     | C    |
| 1   | AA    | 90     | U    |
| 1   | AA    | 91     | C    |
| 1   | AA    | 97     | G    |
| 1   | AA    | 98     | G    |
| 1   | AA    | 101    | A    |
| 1   | AA    | 104    | G    |
| 1   | AA    | 116    | A    |
| 1   | AA    | 120    | A    |
| 1   | AA    | 121    | C    |
| 1   | AA    | 129    | U    |
| 1   | AA    | 129(A) | G    |
| 1   | AA    | 131    | C    |
| 1   | AA    | 144    | G    |
| 1   | AA    | 146    | G    |
| 1   | AA    | 147    | G    |
| 1   | AA    | 149    | A    |
| 1   | AA    | 160    | A    |
| 1   | AA    | 163    | C    |
| 1   | AA    | 181    | G    |
| 1   | AA    | 182    | U    |
| 1   | AA    | 189(G) | G    |
| 1   | AA    | 189(H) | G    |
| 1   | AA    | 195    | A    |
| 1   | AA    | 197    | A    |
| 1   | AA    | 198    | G    |
| 1   | AA    | 202    | U    |
| 1   | AA    | 203    | U    |
| 1   | AA    | 204    | U    |
| 1   | AA    | 216    | G    |
| 1   | AA    | 243    | A    |
| 1   | AA    | 244    | U    |
| 1   | AA    | 247    | G    |
| 1   | AA    | 251    | G    |
| 1   | AA    | 266    | G    |
| 1   | AA    | 267    | C    |
| 1   | AA    | 268    | C    |
| 1   | AA    | 281    | G    |
| 1   | AA    | 289    | G    |
| 1   | AA    | 316    | G    |
| 1   | AA    | 321    | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 328 | C    |
| 1   | AA    | 329 | A    |
| 1   | AA    | 332 | G    |
| 1   | AA    | 344 | A    |
| 1   | AA    | 345 | C    |
| 1   | AA    | 346 | G    |
| 1   | AA    | 350 | G    |
| 1   | AA    | 352 | C    |
| 1   | AA    | 353 | A    |
| 1   | AA    | 354 | G    |
| 1   | AA    | 367 | U    |
| 1   | AA    | 372 | C    |
| 1   | AA    | 397 | A    |
| 1   | AA    | 398 | C    |
| 1   | AA    | 412 | A    |
| 1   | AA    | 413 | G    |
| 1   | AA    | 414 | A    |
| 1   | AA    | 422 | C    |
| 1   | AA    | 428 | G    |
| 1   | AA    | 429 | U    |
| 1   | AA    | 430 | A    |
| 1   | AA    | 435 | C    |
| 1   | AA    | 437 | U    |
| 1   | AA    | 439 | A    |
| 1   | AA    | 444 | C    |
| 1   | AA    | 452 | A    |
| 1   | AA    | 460 | G    |
| 1   | AA    | 461 | A    |
| 1   | AA    | 471 | G    |
| 1   | AA    | 481 | G    |
| 1   | AA    | 484 | G    |
| 1   | AA    | 485 | G    |
| 1   | AA    | 496 | A    |
| 1   | AA    | 498 | U    |
| 1   | AA    | 509 | A    |
| 1   | AA    | 510 | A    |
| 1   | AA    | 511 | C    |
| 1   | AA    | 527 | G    |
| 1   | AA    | 531 | U    |
| 1   | AA    | 532 | A    |
| 1   | AA    | 533 | A    |
| 1   | AA    | 534 | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 536 | C    |
| 1   | AA    | 547 | A    |
| 1   | AA    | 553 | A    |
| 1   | AA    | 559 | A    |
| 1   | AA    | 560 | U    |
| 1   | AA    | 561 | U    |
| 1   | AA    | 562 | C    |
| 1   | AA    | 572 | A    |
| 1   | AA    | 573 | A    |
| 1   | AA    | 575 | G    |
| 1   | AA    | 576 | G    |
| 1   | AA    | 577 | G    |
| 1   | AA    | 588 | G    |
| 1   | AA    | 596 | C    |
| 1   | AA    | 631 | G    |
| 1   | AA    | 632 | A    |
| 1   | AA    | 650 | G    |
| 1   | AA    | 653 | A    |
| 1   | AA    | 665 | A    |
| 1   | AA    | 682 | G    |
| 1   | AA    | 683 | G    |
| 1   | AA    | 686 | U    |
| 1   | AA    | 687 | A    |
| 1   | AA    | 688 | G    |
| 1   | AA    | 704 | A    |
| 1   | AA    | 721 | G    |
| 1   | AA    | 722 | A    |
| 1   | AA    | 723 | U    |
| 1   | AA    | 724 | G    |
| 1   | AA    | 728 | A    |
| 1   | AA    | 731 | G    |
| 1   | AA    | 744 | C    |
| 1   | AA    | 748 | C    |
| 1   | AA    | 755 | G    |
| 1   | AA    | 777 | A    |
| 1   | AA    | 793 | U    |
| 1   | AA    | 794 | A    |
| 1   | AA    | 813 | U    |
| 1   | AA    | 816 | A    |
| 1   | AA    | 817 | C    |
| 1   | AA    | 828 | A    |
| 1   | AA    | 839 | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | AA    | 840     | C    |
| 1   | AA    | 841     | U    |
| 1   | AA    | 848     | C    |
| 1   | AA    | 858     | G    |
| 1   | AA    | 859     | A    |
| 1   | AA    | 867     | G    |
| 1   | AA    | 874     | G    |
| 1   | AA    | 895     | G    |
| 1   | AA    | 907     | A    |
| 1   | AA    | 914     | A    |
| 1   | AA    | 921     | U    |
| 1   | AA    | 927     | G    |
| 1   | AA    | 934     | C    |
| 1   | AA    | 935     | A    |
| 1   | AA    | 951     | G    |
| 1   | AA    | 960     | U    |
| 1   | AA    | 961     | U    |
| 1   | AA    | 968     | A    |
| 1   | AA    | 969     | A    |
| 1   | AA    | 974     | A    |
| 1   | AA    | 975     | A    |
| 1   | AA    | 976     | G    |
| 1   | AA    | 977     | A    |
| 1   | AA    | 978     | A    |
| 1   | AA    | 980     | C    |
| 1   | AA    | 981     | U    |
| 1   | AA    | 991     | U    |
| 1   | AA    | 992     | U    |
| 1   | AA    | 993     | G    |
| 1   | AA    | 997     | U    |
| 1   | AA    | 1003    | G    |
| 1   | AA    | 1004    | A    |
| 1   | AA    | 1005    | A    |
| 1   | AA    | 1010    | G    |
| 1   | AA    | 1027    | C    |
| 1   | AA    | 1030    | C    |
| 1   | AA    | 1030(B) | C    |
| 1   | AA    | 1050    | G    |
| 1   | AA    | 1054    | C    |
| 1   | AA    | 1064    | G    |
| 1   | AA    | 1065    | U    |
| 1   | AA    | 1066    | C    |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AA    | 1068 | G    |
| 1   | AA    | 1094 | G    |
| 1   | AA    | 1095 | U    |
| 1   | AA    | 1101 | A    |
| 1   | AA    | 1102 | A    |
| 1   | AA    | 1117 | G    |
| 1   | AA    | 1124 | G    |
| 1   | AA    | 1125 | U    |
| 1   | AA    | 1129 | C    |
| 1   | AA    | 1130 | A    |
| 1   | AA    | 1137 | C    |
| 1   | AA    | 1138 | G    |
| 1   | AA    | 1139 | G    |
| 1   | AA    | 1146 | A    |
| 1   | AA    | 1152 | A    |
| 1   | AA    | 1154 | G    |
| 1   | AA    | 1159 | U    |
| 1   | AA    | 1184 | G    |
| 1   | AA    | 1187 | G    |
| 1   | AA    | 1196 | U    |
| 1   | AA    | 1197 | G    |
| 1   | AA    | 1199 | U    |
| 1   | AA    | 1202 | G    |
| 1   | AA    | 1212 | U    |
| 1   | AA    | 1214 | C    |
| 1   | AA    | 1217 | C    |
| 1   | AA    | 1225 | A    |
| 1   | AA    | 1226 | C    |
| 1   | AA    | 1227 | A    |
| 1   | AA    | 1238 | A    |
| 1   | AA    | 1240 | U    |
| 1   | AA    | 1241 | G    |
| 1   | AA    | 1249 | C    |
| 1   | AA    | 1256 | A    |
| 1   | AA    | 1257 | U    |
| 1   | AA    | 1273 | G    |
| 1   | AA    | 1280 | A    |
| 1   | AA    | 1281 | U    |
| 1   | AA    | 1285 | A    |
| 1   | AA    | 1286 | A    |
| 1   | AA    | 1287 | A    |
| 1   | AA    | 1298 | C    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | AA    | 1299    | A    |
| 1   | AA    | 1300    | G    |
| 1   | AA    | 1301    | U    |
| 1   | AA    | 1302    | U    |
| 1   | AA    | 1317    | C    |
| 1   | AA    | 1320    | C    |
| 1   | AA    | 1322    | C    |
| 1   | AA    | 1323    | G    |
| 1   | AA    | 1331    | G    |
| 1   | AA    | 1335    | C    |
| 1   | AA    | 1336    | C    |
| 1   | AA    | 1337    | G    |
| 1   | AA    | 1338    | G    |
| 1   | AA    | 1346    | A    |
| 1   | AA    | 1348    | U    |
| 1   | AA    | 1354    | C    |
| 1   | AA    | 1363    | C    |
| 1   | AA    | 1364    | U    |
| 1   | AA    | 1365    | G    |
| 1   | AA    | 1370    | G    |
| 1   | AA    | 1379    | G    |
| 1   | AA    | 1394    | A    |
| 1   | AA    | 1397    | C    |
| 1   | AA    | 1398    | A    |
| 1   | AA    | 1404    | C    |
| 1   | AA    | 1419    | G    |
| 1   | AA    | 1434    | A    |
| 1   | AA    | 1442    | G    |
| 1   | AA    | 1442(A) | G    |
| 1   | AA    | 1443    | G    |
| 1   | AA    | 1447    | A    |
| 1   | AA    | 1452    | C    |
| 1   | AA    | 1456    | G    |
| 1   | AA    | 1490    | C    |
| 1   | AA    | 1492    | A    |
| 1   | AA    | 1493    | A    |
| 1   | AA    | 1494    | G    |
| 1   | AA    | 1499    | A    |
| 1   | AA    | 1503    | A    |
| 1   | AA    | 1504    | G    |
| 1   | AA    | 1505    | G    |
| 1   | AA    | 1506    | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | AA    | 1507  | A    |
| 1   | AA    | 1517  | G    |
| 1   | AA    | 1519  | A    |
| 1   | AA    | 1520  | G    |
| 1   | AA    | 1529  | G    |
| 1   | AA    | 1530  | G    |
| 22  | AV    | 4     | G    |
| 22  | AV    | 5     | G    |
| 22  | AV    | 8     | U    |
| 22  | AV    | 17    | C    |
| 22  | AV    | 17(A) | U    |
| 22  | AV    | 18    | G    |
| 22  | AV    | 19    | G    |
| 22  | AV    | 20    | U    |
| 22  | AV    | 21    | A    |
| 22  | AV    | 47    | U    |
| 22  | AV    | 48    | C    |
| 22  | AV    | 63    | G    |
| 22  | AV    | 71    | C    |
| 22  | AV    | 75    | C    |
| 22  | AV    | 76    | A    |
| 22  | AW    | 5     | G    |
| 22  | AW    | 7     | G    |
| 22  | AW    | 8     | U    |
| 22  | AW    | 9     | G    |
| 22  | AW    | 10    | G    |
| 22  | AW    | 15    | G    |
| 22  | AW    | 18    | U    |
| 22  | AW    | 19    | G    |
| 22  | AW    | 20    | G    |
| 22  | AW    | 21    | U    |
| 22  | AW    | 22    | A    |
| 22  | AW    | 28    | U    |
| 22  | AW    | 48    | U    |
| 22  | AW    | 49    | C    |
| 22  | AW    | 50    | G    |
| 22  | AW    | 53    | G    |
| 22  | AW    | 62    | C    |
| 22  | AW    | 64    | G    |
| 22  | AW    | 66    | C    |
| 22  | AW    | 68    | C    |
| 22  | AW    | 69    | C    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 22  | AW    | 72     | C    |
| 22  | AW    | 73     | A    |
| 22  | AW    | 74     | A    |
| 22  | AW    | 75     | C    |
| 23  | AX    | 12     | A    |
| 23  | AX    | 13     | A    |
| 23  | AX    | 14     | A    |
| 23  | AX    | 19     | U    |
| 35  | BA    | 9      | U    |
| 35  | BA    | 18     | C    |
| 35  | BA    | 28     | A    |
| 35  | BA    | 35     | G    |
| 35  | BA    | 42     | G    |
| 35  | BA    | 43     | A    |
| 35  | BA    | 45     | C    |
| 35  | BA    | 49     | A    |
| 35  | BA    | 50     | U    |
| 35  | BA    | 61     | G    |
| 35  | BA    | 63     | U    |
| 35  | BA    | 72     | U    |
| 35  | BA    | 75     | G    |
| 35  | BA    | 83     | G    |
| 35  | BA    | 84     | A    |
| 35  | BA    | 85     | G    |
| 35  | BA    | 88     | G    |
| 35  | BA    | 90     | U    |
| 35  | BA    | 92     | A    |
| 35  | BA    | 94     | C    |
| 35  | BA    | 95     | G    |
| 35  | BA    | 100    | G    |
| 35  | BA    | 102    | G    |
| 35  | BA    | 106    | C    |
| 35  | BA    | 116    | C    |
| 35  | BA    | 118    | A    |
| 35  | BA    | 119    | A    |
| 35  | BA    | 121    | G    |
| 35  | BA    | 125    | G    |
| 35  | BA    | 129    | C    |
| 35  | BA    | 139(A) | G    |
| 35  | BA    | 141    | A    |
| 35  | BA    | 142(A) | C    |
| 35  | BA    | 155    | U    |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | BA           | 156        | U           |
| 35         | BA           | 157        | U           |
| 35         | BA           | 171        | G           |
| 35         | BA           | 174        | C           |
| 35         | BA           | 190        | A           |
| 35         | BA           | 196        | A           |
| 35         | BA           | 199        | A           |
| 35         | BA           | 204        | A           |
| 35         | BA           | 205        | G           |
| 35         | BA           | 212        | G           |
| 35         | BA           | 215        | G           |
| 35         | BA           | 216        | A           |
| 35         | BA           | 221        | A           |
| 35         | BA           | 222        | A           |
| 35         | BA           | 227        | A           |
| 35         | BA           | 241        | A           |
| 35         | BA           | 248        | G           |
| 35         | BA           | 252        | G           |
| 35         | BA           | 261        | G           |
| 35         | BA           | 271(J)     | C           |
| 35         | BA           | 271(K)     | U           |
| 35         | BA           | 271(L)     | U           |
| 35         | BA           | 271(O)     | C           |
| 35         | BA           | 271(Y)     | U           |
| 35         | BA           | 272        | G           |
| 35         | BA           | 272(A)     | U           |
| 35         | BA           | 272(B)     | G           |
| 35         | BA           | 272(H)     | C           |
| 35         | BA           | 272(I)     | U           |
| 35         | BA           | 276        | A           |
| 35         | BA           | 280        | C           |
| 35         | BA           | 283        | A           |
| 35         | BA           | 286        | C           |
| 35         | BA           | 299        | A           |
| 35         | BA           | 310        | A           |
| 35         | BA           | 311        | A           |
| 35         | BA           | 329        | G           |
| 35         | BA           | 330        | A           |
| 35         | BA           | 332        | A           |
| 35         | BA           | 333        | G           |
| 35         | BA           | 336        | C           |
| 35         | BA           | 345        | A           |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 35  | BA    | 346    | A    |
| 35  | BA    | 352    | G    |
| 35  | BA    | 353    | G    |
| 35  | BA    | 362    | U    |
| 35  | BA    | 363    | G    |
| 35  | BA    | 363(F) | A    |
| 35  | BA    | 364    | C    |
| 35  | BA    | 365    | C    |
| 35  | BA    | 371    | A    |
| 35  | BA    | 372    | G    |
| 35  | BA    | 386    | G    |
| 35  | BA    | 396    | G    |
| 35  | BA    | 405    | U    |
| 35  | BA    | 406    | G    |
| 35  | BA    | 407    | G    |
| 35  | BA    | 411    | G    |
| 35  | BA    | 412    | A    |
| 35  | BA    | 428    | A    |
| 35  | BA    | 444    | C    |
| 35  | BA    | 448    | U    |
| 35  | BA    | 449    | A    |
| 35  | BA    | 455    | C    |
| 35  | BA    | 458    | G    |
| 35  | BA    | 475    | U    |
| 35  | BA    | 480    | A    |
| 35  | BA    | 481    | G    |
| 35  | BA    | 504    | U    |
| 35  | BA    | 505    | A    |
| 35  | BA    | 508    | G    |
| 35  | BA    | 509    | C    |
| 35  | BA    | 526    | A    |
| 35  | BA    | 527    | C    |
| 35  | BA    | 528    | A    |
| 35  | BA    | 529    | A    |
| 35  | BA    | 530    | G    |
| 35  | BA    | 531    | C    |
| 35  | BA    | 532    | A    |
| 35  | BA    | 544    | G    |
| 35  | BA    | 548    | A    |
| 35  | BA    | 552    | G    |
| 35  | BA    | 555    | U    |
| 35  | BA    | 556    | G    |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | BA           | 562        | U           |
| 35         | BA           | 563        | G           |
| 35         | BA           | 573        | G           |
| 35         | BA           | 575        | A           |
| 35         | BA           | 587        | C           |
| 35         | BA           | 591        | C           |
| 35         | BA           | 592        | G           |
| 35         | BA           | 604        | G           |
| 35         | BA           | 607        | U           |
| 35         | BA           | 613        | G           |
| 35         | BA           | 614(B)     | G           |
| 35         | BA           | 615        | G           |
| 35         | BA           | 620        | G           |
| 35         | BA           | 622        | G           |
| 35         | BA           | 627        | A           |
| 35         | BA           | 637        | A           |
| 35         | BA           | 645        | C           |
| 35         | BA           | 646        | A           |
| 35         | BA           | 651        | G           |
| 35         | BA           | 653        | A           |
| 35         | BA           | 654        | A           |
| 35         | BA           | 654(I)     | C           |
| 35         | BA           | 654(J)     | A           |
| 35         | BA           | 654(K)     | C           |
| 35         | BA           | 654(M)     | C           |
| 35         | BA           | 654(T)     | C           |
| 35         | BA           | 655        | A           |
| 35         | BA           | 675        | A           |
| 35         | BA           | 682        | G           |
| 35         | BA           | 686        | G           |
| 35         | BA           | 695        | G           |
| 35         | BA           | 699        | A           |
| 35         | BA           | 722        | A           |
| 35         | BA           | 727        | A           |
| 35         | BA           | 729        | G           |
| 35         | BA           | 730        | C           |
| 35         | BA           | 740        | U           |
| 35         | BA           | 745        | G           |
| 35         | BA           | 753        | C           |
| 35         | BA           | 764        | A           |
| 35         | BA           | 765        | G           |
| 35         | BA           | 775        | G           |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | BA           | 776        | G           |
| 35         | BA           | 782        | A           |
| 35         | BA           | 784        | A           |
| 35         | BA           | 785        | G           |
| 35         | BA           | 788        | A           |
| 35         | BA           | 789        | A           |
| 35         | BA           | 790        | C           |
| 35         | BA           | 791        | C           |
| 35         | BA           | 792        | G           |
| 35         | BA           | 793        | A           |
| 35         | BA           | 794        | G           |
| 35         | BA           | 800        | A           |
| 35         | BA           | 805        | G           |
| 35         | BA           | 811        | U           |
| 35         | BA           | 812        | C           |
| 35         | BA           | 827        | U           |
| 35         | BA           | 828        | U           |
| 35         | BA           | 830        | G           |
| 35         | BA           | 840        | C           |
| 35         | BA           | 841        | A           |
| 35         | BA           | 859        | G           |
| 35         | BA           | 878        | A           |
| 35         | BA           | 889        | C           |
| 35         | BA           | 896        | A           |
| 35         | BA           | 897        | C           |
| 35         | BA           | 900        | A           |
| 35         | BA           | 904        | C           |
| 35         | BA           | 910        | A           |
| 35         | BA           | 926        | A           |
| 35         | BA           | 932        | G           |
| 35         | BA           | 940        | G           |
| 35         | BA           | 941        | A           |
| 35         | BA           | 945        | A           |
| 35         | BA           | 946        | G           |
| 35         | BA           | 959        | A           |
| 35         | BA           | 961        | C           |
| 35         | BA           | 962        | G           |
| 35         | BA           | 969        | U           |
| 35         | BA           | 974        | G           |
| 35         | BA           | 975        | C           |
| 35         | BA           | 980        | A           |
| 35         | BA           | 983        | A           |

*Continued on next page...*



*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | BA           | 985        | C           |
| 35         | BA           | 990        | A           |
| 35         | BA           | 991        | C           |
| 35         | BA           | 996        | A           |
| 35         | BA           | 1005       | C           |
| 35         | BA           | 1011       | G           |
| 35         | BA           | 1012       | U           |
| 35         | BA           | 1013       | C           |
| 35         | BA           | 1021       | A           |
| 35         | BA           | 1022       | G           |
| 35         | BA           | 1023       | U           |
| 35         | BA           | 1026       | U           |
| 35         | BA           | 1033       | U           |
| 35         | BA           | 1034       | G           |
| 35         | BA           | 1039       | G           |
| 35         | BA           | 1044       | G           |
| 35         | BA           | 1045       | A           |
| 35         | BA           | 1047       | G           |
| 35         | BA           | 1048       | A           |
| 35         | BA           | 1049       | C           |
| 35         | BA           | 1052       | C           |
| 35         | BA           | 1053       | C           |
| 35         | BA           | 1054       | A           |
| 35         | BA           | 1058       | G           |
| 35         | BA           | 1062       | G           |
| 35         | BA           | 1067       | A           |
| 35         | BA           | 1070       | A           |
| 35         | BA           | 1073       | A           |
| 35         | BA           | 1076       | C           |
| 35         | BA           | 1088       | A           |
| 35         | BA           | 1090       | U           |
| 35         | BA           | 1109       | C           |
| 35         | BA           | 1111       | A           |
| 35         | BA           | 1112       | G           |
| 35         | BA           | 1114       | G           |
| 35         | BA           | 1115       | G           |
| 35         | BA           | 1122       | G           |
| 35         | BA           | 1126       | A           |
| 35         | BA           | 1135       | C           |
| 35         | BA           | 1136       | G           |
| 35         | BA           | 1141       | U           |
| 35         | BA           | 1142       | U           |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | BA           | 1142(A)    | A           |
| 35         | BA           | 1143       | A           |
| 35         | BA           | 1146       | C           |
| 35         | BA           | 1155       | A           |
| 35         | BA           | 1157       | G           |
| 35         | BA           | 1158       | C           |
| 35         | BA           | 1159       | U           |
| 35         | BA           | 1170       | G           |
| 35         | BA           | 1173       | G           |
| 35         | BA           | 1174       | A           |
| 35         | BA           | 1175       | U           |
| 35         | BA           | 1176       | G           |
| 35         | BA           | 1177       | A           |
| 35         | BA           | 1204       | A           |
| 35         | BA           | 1210       | A           |
| 35         | BA           | 1211       | U           |
| 35         | BA           | 1212       | G           |
| 35         | BA           | 1213       | A           |
| 35         | BA           | 1220       | A           |
| 35         | BA           | 1221       | C           |
| 35         | BA           | 1224       | C           |
| 35         | BA           | 1238       | G           |
| 35         | BA           | 1247       | A           |
| 35         | BA           | 1248       | G           |
| 35         | BA           | 1250       | G           |
| 35         | BA           | 1251       | C           |
| 35         | BA           | 1252       | G           |
| 35         | BA           | 1255       | U           |
| 35         | BA           | 1256       | G           |
| 35         | BA           | 1266       | G           |
| 35         | BA           | 1271       | G           |
| 35         | BA           | 1272       | A           |
| 35         | BA           | 1273       | U           |
| 35         | BA           | 1287       | A           |
| 35         | BA           | 1300       | U           |
| 35         | BA           | 1302       | A           |
| 35         | BA           | 1314       | C           |
| 35         | BA           | 1326       | U           |
| 35         | BA           | 1329       | U           |
| 35         | BA           | 1330       | C           |
| 35         | BA           | 1332       | G           |
| 35         | BA           | 1342       | A           |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | BA           | 1345       | C           |
| 35         | BA           | 1349       | A           |
| 35         | BA           | 1359       | A           |
| 35         | BA           | 1365       | A           |
| 35         | BA           | 1379       | A           |
| 35         | BA           | 1380       | G           |
| 35         | BA           | 1384       | A           |
| 35         | BA           | 1385       | G           |
| 35         | BA           | 1386       | C           |
| 35         | BA           | 1396       | U           |
| 35         | BA           | 1403       | C           |
| 35         | BA           | 1406       | U           |
| 35         | BA           | 1411       | C           |
| 35         | BA           | 1416       | G           |
| 35         | BA           | 1420       | U           |
| 35         | BA           | 1421       | G           |
| 35         | BA           | 1427       | A           |
| 35         | BA           | 1428       | C           |
| 35         | BA           | 1434       | A           |
| 35         | BA           | 1435       | G           |
| 35         | BA           | 1445       | A           |
| 35         | BA           | 1445(A)    | C           |
| 35         | BA           | 1453       | U           |
| 35         | BA           | 1455       | G           |
| 35         | BA           | 1459       | G           |
| 35         | BA           | 1460       | A           |
| 35         | BA           | 1461       | G           |
| 35         | BA           | 1467       | C           |
| 35         | BA           | 1476       | C           |
| 35         | BA           | 1477       | A           |
| 35         | BA           | 1478       | G           |
| 35         | BA           | 1482       | G           |
| 35         | BA           | 1484       | G           |
| 35         | BA           | 1485       | G           |
| 35         | BA           | 1488       | G           |
| 35         | BA           | 1490       | A           |
| 35         | BA           | 1491       | G           |
| 35         | BA           | 1493       | C           |
| 35         | BA           | 1494       | A           |
| 35         | BA           | 1495       | A           |
| 35         | BA           | 1496       | A           |
| 35         | BA           | 1497       | U           |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | BA           | 1505       | C           |
| 35         | BA           | 1509       | C           |
| 35         | BA           | 1509(A)    | A           |
| 35         | BA           | 1517       | G           |
| 35         | BA           | 1528(A)    | A           |
| 35         | BA           | 1541       | G           |
| 35         | BA           | 1542       | A           |
| 35         | BA           | 1544       | A           |
| 35         | BA           | 1553       | A           |
| 35         | BA           | 1554       | A           |
| 35         | BA           | 1559       | G           |
| 35         | BA           | 1569       | A           |
| 35         | BA           | 1578       | U           |
| 35         | BA           | 1579       | A           |
| 35         | BA           | 1584       | C           |
| 35         | BA           | 1586       | A           |
| 35         | BA           | 1588       | C           |
| 35         | BA           | 1603       | A           |
| 35         | BA           | 1608       | A           |
| 35         | BA           | 1609       | A           |
| 35         | BA           | 1610       | A           |
| 35         | BA           | 1615       | C           |
| 35         | BA           | 1616       | A           |
| 35         | BA           | 1618       | A           |
| 35         | BA           | 1634       | A           |
| 35         | BA           | 1640       | C           |
| 35         | BA           | 1644       | C           |
| 35         | BA           | 1648       | C           |
| 35         | BA           | 1668       | A           |
| 35         | BA           | 1674       | G           |
| 35         | BA           | 1678       | G           |
| 35         | BA           | 1698       | A           |
| 35         | BA           | 1699       | G           |
| 35         | BA           | 1718       | G           |
| 35         | BA           | 1722       | A           |
| 35         | BA           | 1739       | U           |
| 35         | BA           | 1740       | G           |
| 35         | BA           | 1744       | C           |
| 35         | BA           | 1748       | G           |
| 35         | BA           | 1763       | G           |
| 35         | BA           | 1764       | G           |
| 35         | BA           | 1773       | A           |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | BA           | 1780       | A           |
| 35         | BA           | 1781       | C           |
| 35         | BA           | 1784       | A           |
| 35         | BA           | 1787       | A           |
| 35         | BA           | 1791       | A           |
| 35         | BA           | 1799       | G           |
| 35         | BA           | 1800       | C           |
| 35         | BA           | 1801       | G           |
| 35         | BA           | 1815       | A           |
| 35         | BA           | 1816       | G           |
| 35         | BA           | 1820       | U           |
| 35         | BA           | 1821       | A           |
| 35         | BA           | 1829       | A           |
| 35         | BA           | 1839       | G           |
| 35         | BA           | 1846       | G           |
| 35         | BA           | 1847       | A           |
| 35         | BA           | 1850       | G           |
| 35         | BA           | 1858       | G           |
| 35         | BA           | 1862       | G           |
| 35         | BA           | 1866       | C           |
| 35         | BA           | 1878       | G           |
| 35         | BA           | 1885       | A           |
| 35         | BA           | 1888       | G           |
| 35         | BA           | 1889       | A           |
| 35         | BA           | 1900       | A           |
| 35         | BA           | 1906       | G           |
| 35         | BA           | 1912       | A           |
| 35         | BA           | 1929       | G           |
| 35         | BA           | 1930       | G           |
| 35         | BA           | 1931       | U           |
| 35         | BA           | 1937       | A           |
| 35         | BA           | 1938       | A           |
| 35         | BA           | 1943       | U           |
| 35         | BA           | 1944       | U           |
| 35         | BA           | 1945       | G           |
| 35         | BA           | 1948       | G           |
| 35         | BA           | 1955       | U           |
| 35         | BA           | 1960       | A           |
| 35         | BA           | 1963       | U           |
| 35         | BA           | 1964       | G           |
| 35         | BA           | 1967       | C           |
| 35         | BA           | 1969       | A           |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | BA           | 1970       | A           |
| 35         | BA           | 1971       | A           |
| 35         | BA           | 1972       | A           |
| 35         | BA           | 1987       | G           |
| 35         | BA           | 1993       | U           |
| 35         | BA           | 1997       | G           |
| 35         | BA           | 2004       | G           |
| 35         | BA           | 2021       | C           |
| 35         | BA           | 2022       | U           |
| 35         | BA           | 2023       | G           |
| 35         | BA           | 2031       | A           |
| 35         | BA           | 2033       | A           |
| 35         | BA           | 2034       | U           |
| 35         | BA           | 2043       | C           |
| 35         | BA           | 2055       | C           |
| 35         | BA           | 2056       | G           |
| 35         | BA           | 2060       | A           |
| 35         | BA           | 2061       | G           |
| 35         | BA           | 2062       | A           |
| 35         | BA           | 2065       | C           |
| 35         | BA           | 2069       | G           |
| 35         | BA           | 2076       | U           |
| 35         | BA           | 2100       | G           |
| 35         | BA           | 2103       | C           |
| 35         | BA           | 2104       | G           |
| 35         | BA           | 2112       | G           |
| 35         | BA           | 2116       | G           |
| 35         | BA           | 2118       | U           |
| 35         | BA           | 2127       | G           |
| 35         | BA           | 2131       | G           |
| 35         | BA           | 2132       | U           |
| 35         | BA           | 2133       | G           |
| 35         | BA           | 2134       | A           |
| 35         | BA           | 2157       | G           |
| 35         | BA           | 2158       | A           |
| 35         | BA           | 2159       | G           |
| 35         | BA           | 2163       | C           |
| 35         | BA           | 2172       | U           |
| 35         | BA           | 2173       | A           |
| 35         | BA           | 2185       | C           |
| 35         | BA           | 2187       | G           |
| 35         | BA           | 2189       | U           |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | BA           | 2190       | G           |
| 35         | BA           | 2192       | G           |
| 35         | BA           | 2193       | G           |
| 35         | BA           | 2198       | A           |
| 35         | BA           | 2199       | A           |
| 35         | BA           | 2200       | C           |
| 35         | BA           | 2202       | C           |
| 35         | BA           | 2203       | U           |
| 35         | BA           | 2205       | C           |
| 35         | BA           | 2206       | G           |
| 35         | BA           | 2207       | G           |
| 35         | BA           | 2208       | A           |
| 35         | BA           | 2219       | G           |
| 35         | BA           | 2225       | A           |
| 35         | BA           | 2226       | C           |
| 35         | BA           | 2238       | G           |
| 35         | BA           | 2239       | G           |
| 35         | BA           | 2263       | C           |
| 35         | BA           | 2273       | A           |
| 35         | BA           | 2283       | C           |
| 35         | BA           | 2286       | A           |
| 35         | BA           | 2288       | A           |
| 35         | BA           | 2297       | C           |
| 35         | BA           | 2302       | G           |
| 35         | BA           | 2305       | A           |
| 35         | BA           | 2306       | C           |
| 35         | BA           | 2307       | G           |
| 35         | BA           | 2308       | G           |
| 35         | BA           | 2309       | A           |
| 35         | BA           | 2313       | C           |
| 35         | BA           | 2319       | G           |
| 35         | BA           | 2320       | A           |
| 35         | BA           | 2325       | G           |
| 35         | BA           | 2334       | G           |
| 35         | BA           | 2336       | A           |
| 35         | BA           | 2345       | G           |
| 35         | BA           | 2346       | A           |
| 35         | BA           | 2347       | C           |
| 35         | BA           | 2348       | U           |
| 35         | BA           | 2349       | G           |
| 35         | BA           | 2350       | C           |
| 35         | BA           | 2383       | G           |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | BA           | 2385       | C           |
| 35         | BA           | 2402       | C           |
| 35         | BA           | 2406       | U           |
| 35         | BA           | 2423       | U           |
| 35         | BA           | 2424       | C           |
| 35         | BA           | 2425       | A           |
| 35         | BA           | 2427       | C           |
| 35         | BA           | 2428       | G           |
| 35         | BA           | 2429       | G           |
| 35         | BA           | 2430       | A           |
| 35         | BA           | 2431       | U           |
| 35         | BA           | 2434       | A           |
| 35         | BA           | 2435       | A           |
| 35         | BA           | 2439       | A           |
| 35         | BA           | 2441       | C           |
| 35         | BA           | 2448       | A           |
| 35         | BA           | 2461       | C           |
| 35         | BA           | 2465       | C           |
| 35         | BA           | 2469       | A           |
| 35         | BA           | 2470       | G           |
| 35         | BA           | 2473       | U           |
| 35         | BA           | 2474       | C           |
| 35         | BA           | 2475       | C           |
| 35         | BA           | 2476       | A           |
| 35         | BA           | 2477       | C           |
| 35         | BA           | 2478       | A           |
| 35         | BA           | 2482       | G           |
| 35         | BA           | 2484       | G           |
| 35         | BA           | 2502       | G           |
| 35         | BA           | 2503       | A           |
| 35         | BA           | 2505       | G           |
| 35         | BA           | 2519       | U           |
| 35         | BA           | 2520       | C           |
| 35         | BA           | 2524       | G           |
| 35         | BA           | 2529       | G           |
| 35         | BA           | 2543       | G           |
| 35         | BA           | 2554       | U           |
| 35         | BA           | 2566       | A           |
| 35         | BA           | 2567       | G           |
| 35         | BA           | 2572       | A           |
| 35         | BA           | 2577       | A           |
| 35         | BA           | 2585       | U           |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 35  | BA    | 2586    | C    |
| 35  | BA    | 2602    | A    |
| 35  | BA    | 2609    | U    |
| 35  | BA    | 2610    | C    |
| 35  | BA    | 2611    | U    |
| 35  | BA    | 2612    | C    |
| 35  | BA    | 2615    | U    |
| 35  | BA    | 2630    | G    |
| 35  | BA    | 2646    | C    |
| 35  | BA    | 2655    | G    |
| 35  | BA    | 2657    | A    |
| 35  | BA    | 2658    | C    |
| 35  | BA    | 2670    | A    |
| 35  | BA    | 2673    | G    |
| 35  | BA    | 2682    | U    |
| 35  | BA    | 2690    | C    |
| 35  | BA    | 2691    | C    |
| 35  | BA    | 2702    | U    |
| 35  | BA    | 2703    | C    |
| 35  | BA    | 2706    | G    |
| 35  | BA    | 2712    | U    |
| 35  | BA    | 2712(A) | A    |
| 35  | BA    | 2713    | A    |
| 35  | BA    | 2726    | U    |
| 35  | BA    | 2733    | A    |
| 35  | BA    | 2750    | A    |
| 35  | BA    | 2751    | G    |
| 35  | BA    | 2755    | C    |
| 35  | BA    | 2756    | U    |
| 35  | BA    | 2757    | A    |
| 35  | BA    | 2758    | A    |
| 35  | BA    | 2762    | G    |
| 35  | BA    | 2764    | A    |
| 35  | BA    | 2765    | A    |
| 35  | BA    | 2766    | G    |
| 35  | BA    | 2778    | A    |
| 35  | BA    | 2779    | U    |
| 35  | BA    | 2780    | G    |
| 35  | BA    | 2790    | A    |
| 35  | BA    | 2791    | C    |
| 35  | BA    | 2796    | U    |
| 35  | BA    | 2799    | C    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 35  | BA    | 2801 | A    |
| 35  | BA    | 2802 | G    |
| 35  | BA    | 2803 | C    |
| 35  | BA    | 2808 | U    |
| 35  | BA    | 2820 | A    |
| 35  | BA    | 2821 | A    |
| 35  | BA    | 2824 | C    |
| 35  | BA    | 2833 | G    |
| 35  | BA    | 2834 | G    |
| 35  | BA    | 2836 | U    |
| 35  | BA    | 2849 | U    |
| 35  | BA    | 2872 | G    |
| 35  | BA    | 2879 | C    |
| 35  | BA    | 2880 | C    |
| 35  | BA    | 2892 | A    |
| 35  | BA    | 2894 | G    |
| 35  | BA    | 2895 | U    |
| 36  | BB    | 8    | U    |
| 36  | BB    | 13   | A    |
| 36  | BB    | 15   | A    |
| 36  | BB    | 16   | G    |
| 36  | BB    | 22   | U    |
| 36  | BB    | 25   | A    |
| 36  | BB    | 33   | G    |
| 36  | BB    | 35   | U    |
| 36  | BB    | 41   | U    |
| 36  | BB    | 42   | C    |
| 36  | BB    | 45   | A    |
| 36  | BB    | 52   | A    |
| 36  | BB    | 53   | A    |
| 36  | BB    | 56   | G    |
| 36  | BB    | 67   | G    |
| 36  | BB    | 73   | A    |
| 36  | BB    | 81   | G    |
| 36  | BB    | 82   | G    |
| 36  | BB    | 88   | C    |
| 36  | BB    | 89   | G    |
| 36  | BB    | 90   | A    |
| 36  | BB    | 103  | G    |
| 36  | BB    | 104  | U    |
| 36  | BB    | 110  | G    |
| 36  | BB    | 113  | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | CA    | 9      | G    |
| 1   | CA    | 31     | G    |
| 1   | CA    | 32     | A    |
| 1   | CA    | 33     | A    |
| 1   | CA    | 39     | G    |
| 1   | CA    | 47     | C    |
| 1   | CA    | 48     | C    |
| 1   | CA    | 51     | A    |
| 1   | CA    | 60     | A    |
| 1   | CA    | 61     | G    |
| 1   | CA    | 62     | U    |
| 1   | CA    | 81     | U    |
| 1   | CA    | 88     | A    |
| 1   | CA    | 89     | C    |
| 1   | CA    | 90     | U    |
| 1   | CA    | 91     | C    |
| 1   | CA    | 97     | G    |
| 1   | CA    | 98     | G    |
| 1   | CA    | 101    | A    |
| 1   | CA    | 104    | G    |
| 1   | CA    | 116    | A    |
| 1   | CA    | 120    | A    |
| 1   | CA    | 121    | C    |
| 1   | CA    | 129    | U    |
| 1   | CA    | 129(A) | G    |
| 1   | CA    | 131    | C    |
| 1   | CA    | 144    | G    |
| 1   | CA    | 146    | G    |
| 1   | CA    | 147    | G    |
| 1   | CA    | 149    | A    |
| 1   | CA    | 160    | A    |
| 1   | CA    | 163    | C    |
| 1   | CA    | 181    | G    |
| 1   | CA    | 182    | U    |
| 1   | CA    | 189(G) | G    |
| 1   | CA    | 189(H) | G    |
| 1   | CA    | 195    | A    |
| 1   | CA    | 197    | A    |
| 1   | CA    | 198    | G    |
| 1   | CA    | 202    | U    |
| 1   | CA    | 203    | U    |
| 1   | CA    | 204    | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CA    | 216 | G    |
| 1   | CA    | 243 | A    |
| 1   | CA    | 244 | U    |
| 1   | CA    | 247 | G    |
| 1   | CA    | 251 | G    |
| 1   | CA    | 266 | G    |
| 1   | CA    | 267 | C    |
| 1   | CA    | 268 | C    |
| 1   | CA    | 281 | G    |
| 1   | CA    | 289 | G    |
| 1   | CA    | 316 | G    |
| 1   | CA    | 321 | A    |
| 1   | CA    | 328 | C    |
| 1   | CA    | 329 | A    |
| 1   | CA    | 332 | G    |
| 1   | CA    | 344 | A    |
| 1   | CA    | 345 | C    |
| 1   | CA    | 346 | G    |
| 1   | CA    | 350 | G    |
| 1   | CA    | 352 | C    |
| 1   | CA    | 353 | A    |
| 1   | CA    | 354 | G    |
| 1   | CA    | 367 | U    |
| 1   | CA    | 372 | C    |
| 1   | CA    | 397 | A    |
| 1   | CA    | 398 | C    |
| 1   | CA    | 412 | A    |
| 1   | CA    | 413 | G    |
| 1   | CA    | 414 | A    |
| 1   | CA    | 422 | C    |
| 1   | CA    | 428 | G    |
| 1   | CA    | 429 | U    |
| 1   | CA    | 430 | A    |
| 1   | CA    | 435 | C    |
| 1   | CA    | 437 | U    |
| 1   | CA    | 439 | A    |
| 1   | CA    | 444 | C    |
| 1   | CA    | 452 | A    |
| 1   | CA    | 460 | G    |
| 1   | CA    | 461 | A    |
| 1   | CA    | 471 | G    |
| 1   | CA    | 481 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CA    | 484 | G    |
| 1   | CA    | 485 | G    |
| 1   | CA    | 496 | A    |
| 1   | CA    | 498 | U    |
| 1   | CA    | 509 | A    |
| 1   | CA    | 510 | A    |
| 1   | CA    | 511 | C    |
| 1   | CA    | 527 | G    |
| 1   | CA    | 531 | U    |
| 1   | CA    | 532 | A    |
| 1   | CA    | 533 | A    |
| 1   | CA    | 534 | U    |
| 1   | CA    | 536 | C    |
| 1   | CA    | 547 | A    |
| 1   | CA    | 559 | A    |
| 1   | CA    | 560 | U    |
| 1   | CA    | 561 | U    |
| 1   | CA    | 562 | C    |
| 1   | CA    | 572 | A    |
| 1   | CA    | 573 | A    |
| 1   | CA    | 575 | G    |
| 1   | CA    | 576 | G    |
| 1   | CA    | 577 | G    |
| 1   | CA    | 588 | G    |
| 1   | CA    | 596 | C    |
| 1   | CA    | 631 | G    |
| 1   | CA    | 632 | A    |
| 1   | CA    | 650 | G    |
| 1   | CA    | 653 | A    |
| 1   | CA    | 665 | A    |
| 1   | CA    | 682 | G    |
| 1   | CA    | 683 | G    |
| 1   | CA    | 686 | U    |
| 1   | CA    | 687 | A    |
| 1   | CA    | 688 | G    |
| 1   | CA    | 704 | A    |
| 1   | CA    | 721 | G    |
| 1   | CA    | 722 | A    |
| 1   | CA    | 723 | U    |
| 1   | CA    | 724 | G    |
| 1   | CA    | 728 | A    |
| 1   | CA    | 731 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | CA    | 744  | C    |
| 1   | CA    | 748  | C    |
| 1   | CA    | 755  | G    |
| 1   | CA    | 777  | A    |
| 1   | CA    | 793  | U    |
| 1   | CA    | 794  | A    |
| 1   | CA    | 813  | U    |
| 1   | CA    | 816  | A    |
| 1   | CA    | 817  | C    |
| 1   | CA    | 828  | A    |
| 1   | CA    | 839  | U    |
| 1   | CA    | 840  | C    |
| 1   | CA    | 841  | U    |
| 1   | CA    | 848  | C    |
| 1   | CA    | 858  | G    |
| 1   | CA    | 859  | A    |
| 1   | CA    | 867  | G    |
| 1   | CA    | 874  | G    |
| 1   | CA    | 895  | G    |
| 1   | CA    | 907  | A    |
| 1   | CA    | 914  | A    |
| 1   | CA    | 921  | U    |
| 1   | CA    | 927  | G    |
| 1   | CA    | 934  | C    |
| 1   | CA    | 935  | A    |
| 1   | CA    | 951  | G    |
| 1   | CA    | 960  | U    |
| 1   | CA    | 961  | U    |
| 1   | CA    | 968  | A    |
| 1   | CA    | 969  | A    |
| 1   | CA    | 974  | A    |
| 1   | CA    | 975  | A    |
| 1   | CA    | 976  | G    |
| 1   | CA    | 977  | A    |
| 1   | CA    | 978  | A    |
| 1   | CA    | 980  | C    |
| 1   | CA    | 981  | U    |
| 1   | CA    | 991  | U    |
| 1   | CA    | 992  | U    |
| 1   | CA    | 993  | G    |
| 1   | CA    | 997  | U    |
| 1   | CA    | 1003 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | CA    | 1004    | A    |
| 1   | CA    | 1005    | A    |
| 1   | CA    | 1010    | G    |
| 1   | CA    | 1027    | C    |
| 1   | CA    | 1030    | C    |
| 1   | CA    | 1030(B) | C    |
| 1   | CA    | 1050    | G    |
| 1   | CA    | 1054    | C    |
| 1   | CA    | 1064    | G    |
| 1   | CA    | 1065    | U    |
| 1   | CA    | 1066    | C    |
| 1   | CA    | 1068    | G    |
| 1   | CA    | 1094    | G    |
| 1   | CA    | 1095    | U    |
| 1   | CA    | 1101    | A    |
| 1   | CA    | 1102    | A    |
| 1   | CA    | 1117    | G    |
| 1   | CA    | 1124    | G    |
| 1   | CA    | 1125    | U    |
| 1   | CA    | 1129    | C    |
| 1   | CA    | 1130    | A    |
| 1   | CA    | 1137    | C    |
| 1   | CA    | 1138    | G    |
| 1   | CA    | 1139    | G    |
| 1   | CA    | 1146    | A    |
| 1   | CA    | 1152    | A    |
| 1   | CA    | 1154    | G    |
| 1   | CA    | 1159    | U    |
| 1   | CA    | 1184    | G    |
| 1   | CA    | 1187    | G    |
| 1   | CA    | 1196    | U    |
| 1   | CA    | 1197    | G    |
| 1   | CA    | 1199    | U    |
| 1   | CA    | 1202    | G    |
| 1   | CA    | 1212    | U    |
| 1   | CA    | 1214    | C    |
| 1   | CA    | 1217    | C    |
| 1   | CA    | 1225    | A    |
| 1   | CA    | 1226    | C    |
| 1   | CA    | 1227    | A    |
| 1   | CA    | 1238    | A    |
| 1   | CA    | 1240    | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | CA    | 1241    | G    |
| 1   | CA    | 1249    | C    |
| 1   | CA    | 1256    | A    |
| 1   | CA    | 1257    | U    |
| 1   | CA    | 1273    | G    |
| 1   | CA    | 1280    | A    |
| 1   | CA    | 1281    | U    |
| 1   | CA    | 1285    | A    |
| 1   | CA    | 1286    | A    |
| 1   | CA    | 1287    | A    |
| 1   | CA    | 1298    | C    |
| 1   | CA    | 1299    | A    |
| 1   | CA    | 1300    | G    |
| 1   | CA    | 1301    | U    |
| 1   | CA    | 1302    | U    |
| 1   | CA    | 1317    | C    |
| 1   | CA    | 1322    | C    |
| 1   | CA    | 1323    | G    |
| 1   | CA    | 1331    | G    |
| 1   | CA    | 1335    | C    |
| 1   | CA    | 1336    | C    |
| 1   | CA    | 1337    | G    |
| 1   | CA    | 1338    | G    |
| 1   | CA    | 1346    | A    |
| 1   | CA    | 1348    | U    |
| 1   | CA    | 1354    | C    |
| 1   | CA    | 1363    | C    |
| 1   | CA    | 1364    | U    |
| 1   | CA    | 1365    | G    |
| 1   | CA    | 1370    | G    |
| 1   | CA    | 1379    | G    |
| 1   | CA    | 1394    | A    |
| 1   | CA    | 1397    | C    |
| 1   | CA    | 1398    | A    |
| 1   | CA    | 1404    | C    |
| 1   | CA    | 1419    | G    |
| 1   | CA    | 1442    | G    |
| 1   | CA    | 1442(A) | G    |
| 1   | CA    | 1447    | A    |
| 1   | CA    | 1452    | C    |
| 1   | CA    | 1456    | G    |
| 1   | CA    | 1490    | C    |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | CA    | 1492  | A    |
| 1   | CA    | 1493  | A    |
| 1   | CA    | 1494  | G    |
| 1   | CA    | 1498  | U    |
| 1   | CA    | 1499  | A    |
| 1   | CA    | 1503  | A    |
| 1   | CA    | 1504  | G    |
| 1   | CA    | 1505  | G    |
| 1   | CA    | 1506  | U    |
| 1   | CA    | 1517  | G    |
| 1   | CA    | 1519  | A    |
| 1   | CA    | 1520  | G    |
| 1   | CA    | 1529  | G    |
| 1   | CA    | 1530  | G    |
| 22  | CV    | 3     | C    |
| 22  | CV    | 4     | G    |
| 22  | CV    | 5     | G    |
| 22  | CV    | 17    | C    |
| 22  | CV    | 17(A) | U    |
| 22  | CV    | 18    | G    |
| 22  | CV    | 19    | G    |
| 22  | CV    | 20    | U    |
| 22  | CV    | 21    | A    |
| 22  | CV    | 47    | U    |
| 22  | CV    | 48    | C    |
| 22  | CV    | 63    | G    |
| 22  | CV    | 75    | C    |
| 22  | CV    | 76    | A    |
| 22  | CW    | 4     | G    |
| 22  | CW    | 5     | G    |
| 22  | CW    | 7     | G    |
| 22  | CW    | 9     | G    |
| 22  | CW    | 10    | G    |
| 22  | CW    | 15    | G    |
| 22  | CW    | 18    | U    |
| 22  | CW    | 19    | G    |
| 22  | CW    | 20    | G    |
| 22  | CW    | 21    | U    |
| 22  | CW    | 22    | A    |
| 22  | CW    | 48    | U    |
| 22  | CW    | 49    | C    |
| 22  | CW    | 53    | G    |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 22         | CW           | 66         | C           |
| 22         | CW           | 72         | C           |
| 22         | CW           | 73         | A           |
| 22         | CW           | 74         | A           |
| 22         | CW           | 75         | C           |
| 23         | CX           | 12         | A           |
| 23         | CX           | 13         | A           |
| 23         | CX           | 14         | A           |
| 23         | CX           | 19         | U           |
| 35         | DA           | 9          | U           |
| 35         | DA           | 18         | C           |
| 35         | DA           | 28         | A           |
| 35         | DA           | 35         | G           |
| 35         | DA           | 42         | G           |
| 35         | DA           | 43         | A           |
| 35         | DA           | 45         | C           |
| 35         | DA           | 49         | A           |
| 35         | DA           | 50         | U           |
| 35         | DA           | 61         | G           |
| 35         | DA           | 63         | U           |
| 35         | DA           | 72         | U           |
| 35         | DA           | 75         | G           |
| 35         | DA           | 83         | G           |
| 35         | DA           | 84         | A           |
| 35         | DA           | 85         | G           |
| 35         | DA           | 88         | G           |
| 35         | DA           | 90         | U           |
| 35         | DA           | 92         | A           |
| 35         | DA           | 94         | C           |
| 35         | DA           | 95         | G           |
| 35         | DA           | 100        | G           |
| 35         | DA           | 102        | G           |
| 35         | DA           | 106        | C           |
| 35         | DA           | 116        | C           |
| 35         | DA           | 118        | A           |
| 35         | DA           | 119        | A           |
| 35         | DA           | 121        | G           |
| 35         | DA           | 125        | G           |
| 35         | DA           | 129        | C           |
| 35         | DA           | 139(A)     | G           |
| 35         | DA           | 141        | A           |
| 35         | DA           | 142(A)     | C           |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | DA           | 155        | U           |
| 35         | DA           | 156        | U           |
| 35         | DA           | 157        | U           |
| 35         | DA           | 171        | G           |
| 35         | DA           | 174        | C           |
| 35         | DA           | 190        | A           |
| 35         | DA           | 196        | A           |
| 35         | DA           | 199        | A           |
| 35         | DA           | 204        | A           |
| 35         | DA           | 205        | G           |
| 35         | DA           | 212        | G           |
| 35         | DA           | 215        | G           |
| 35         | DA           | 216        | A           |
| 35         | DA           | 221        | A           |
| 35         | DA           | 222        | A           |
| 35         | DA           | 227        | A           |
| 35         | DA           | 241        | A           |
| 35         | DA           | 248        | G           |
| 35         | DA           | 252        | G           |
| 35         | DA           | 261        | G           |
| 35         | DA           | 271(J)     | C           |
| 35         | DA           | 271(K)     | U           |
| 35         | DA           | 271(L)     | U           |
| 35         | DA           | 271(O)     | C           |
| 35         | DA           | 271(Y)     | U           |
| 35         | DA           | 272        | G           |
| 35         | DA           | 272(A)     | U           |
| 35         | DA           | 272(B)     | G           |
| 35         | DA           | 272(H)     | C           |
| 35         | DA           | 272(I)     | U           |
| 35         | DA           | 276        | A           |
| 35         | DA           | 280        | C           |
| 35         | DA           | 283        | A           |
| 35         | DA           | 286        | C           |
| 35         | DA           | 299        | A           |
| 35         | DA           | 310        | A           |
| 35         | DA           | 311        | A           |
| 35         | DA           | 329        | G           |
| 35         | DA           | 330        | A           |
| 35         | DA           | 332        | A           |
| 35         | DA           | 333        | G           |
| 35         | DA           | 336        | C           |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 35  | DA    | 345    | A    |
| 35  | DA    | 346    | A    |
| 35  | DA    | 352    | G    |
| 35  | DA    | 353    | G    |
| 35  | DA    | 362    | U    |
| 35  | DA    | 363    | G    |
| 35  | DA    | 363(F) | A    |
| 35  | DA    | 364    | C    |
| 35  | DA    | 365    | C    |
| 35  | DA    | 371    | A    |
| 35  | DA    | 372    | G    |
| 35  | DA    | 386    | G    |
| 35  | DA    | 396    | G    |
| 35  | DA    | 405    | U    |
| 35  | DA    | 406    | G    |
| 35  | DA    | 407    | G    |
| 35  | DA    | 411    | G    |
| 35  | DA    | 412    | A    |
| 35  | DA    | 428    | A    |
| 35  | DA    | 444    | C    |
| 35  | DA    | 448    | U    |
| 35  | DA    | 449    | A    |
| 35  | DA    | 455    | C    |
| 35  | DA    | 458    | G    |
| 35  | DA    | 475    | U    |
| 35  | DA    | 480    | A    |
| 35  | DA    | 481    | G    |
| 35  | DA    | 504    | U    |
| 35  | DA    | 505    | A    |
| 35  | DA    | 508    | G    |
| 35  | DA    | 509    | C    |
| 35  | DA    | 526    | A    |
| 35  | DA    | 527    | C    |
| 35  | DA    | 528    | A    |
| 35  | DA    | 529    | A    |
| 35  | DA    | 530    | G    |
| 35  | DA    | 531    | C    |
| 35  | DA    | 532    | A    |
| 35  | DA    | 544    | G    |
| 35  | DA    | 548    | A    |
| 35  | DA    | 552    | G    |
| 35  | DA    | 555    | U    |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | DA           | 556        | G           |
| 35         | DA           | 562        | U           |
| 35         | DA           | 563        | G           |
| 35         | DA           | 573        | G           |
| 35         | DA           | 575        | A           |
| 35         | DA           | 587        | C           |
| 35         | DA           | 591        | C           |
| 35         | DA           | 592        | G           |
| 35         | DA           | 604        | G           |
| 35         | DA           | 607        | U           |
| 35         | DA           | 613        | G           |
| 35         | DA           | 614(B)     | G           |
| 35         | DA           | 615        | G           |
| 35         | DA           | 620        | G           |
| 35         | DA           | 622        | G           |
| 35         | DA           | 627        | A           |
| 35         | DA           | 637        | A           |
| 35         | DA           | 645        | C           |
| 35         | DA           | 646        | A           |
| 35         | DA           | 651        | G           |
| 35         | DA           | 653        | A           |
| 35         | DA           | 654        | A           |
| 35         | DA           | 654(I)     | C           |
| 35         | DA           | 654(J)     | A           |
| 35         | DA           | 654(K)     | C           |
| 35         | DA           | 654(M)     | C           |
| 35         | DA           | 654(T)     | C           |
| 35         | DA           | 655        | A           |
| 35         | DA           | 675        | A           |
| 35         | DA           | 682        | G           |
| 35         | DA           | 686        | G           |
| 35         | DA           | 695        | G           |
| 35         | DA           | 699        | A           |
| 35         | DA           | 722        | A           |
| 35         | DA           | 727        | A           |
| 35         | DA           | 729        | G           |
| 35         | DA           | 730        | C           |
| 35         | DA           | 740        | U           |
| 35         | DA           | 745        | G           |
| 35         | DA           | 753        | C           |
| 35         | DA           | 764        | A           |
| 35         | DA           | 765        | G           |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | DA           | 775        | G           |
| 35         | DA           | 776        | G           |
| 35         | DA           | 782        | A           |
| 35         | DA           | 784        | A           |
| 35         | DA           | 785        | G           |
| 35         | DA           | 788        | A           |
| 35         | DA           | 789        | A           |
| 35         | DA           | 790        | C           |
| 35         | DA           | 791        | C           |
| 35         | DA           | 792        | G           |
| 35         | DA           | 793        | A           |
| 35         | DA           | 794        | G           |
| 35         | DA           | 800        | A           |
| 35         | DA           | 805        | G           |
| 35         | DA           | 811        | U           |
| 35         | DA           | 812        | C           |
| 35         | DA           | 827        | U           |
| 35         | DA           | 828        | U           |
| 35         | DA           | 830        | G           |
| 35         | DA           | 840        | C           |
| 35         | DA           | 841        | A           |
| 35         | DA           | 859        | G           |
| 35         | DA           | 878        | A           |
| 35         | DA           | 889        | C           |
| 35         | DA           | 896        | A           |
| 35         | DA           | 897        | C           |
| 35         | DA           | 900        | A           |
| 35         | DA           | 904        | C           |
| 35         | DA           | 910        | A           |
| 35         | DA           | 926        | A           |
| 35         | DA           | 932        | G           |
| 35         | DA           | 940        | G           |
| 35         | DA           | 941        | A           |
| 35         | DA           | 945        | A           |
| 35         | DA           | 946        | G           |
| 35         | DA           | 959        | A           |
| 35         | DA           | 961        | C           |
| 35         | DA           | 962        | G           |
| 35         | DA           | 969        | U           |
| 35         | DA           | 974        | G           |
| 35         | DA           | 975        | C           |
| 35         | DA           | 980        | A           |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | DA           | 983        | A           |
| 35         | DA           | 985        | C           |
| 35         | DA           | 990        | A           |
| 35         | DA           | 991        | C           |
| 35         | DA           | 996        | A           |
| 35         | DA           | 1005       | C           |
| 35         | DA           | 1011       | G           |
| 35         | DA           | 1012       | U           |
| 35         | DA           | 1013       | C           |
| 35         | DA           | 1021       | A           |
| 35         | DA           | 1022       | G           |
| 35         | DA           | 1023       | U           |
| 35         | DA           | 1026       | U           |
| 35         | DA           | 1033       | U           |
| 35         | DA           | 1034       | G           |
| 35         | DA           | 1039       | G           |
| 35         | DA           | 1044       | G           |
| 35         | DA           | 1045       | A           |
| 35         | DA           | 1047       | G           |
| 35         | DA           | 1048       | A           |
| 35         | DA           | 1049       | C           |
| 35         | DA           | 1052       | C           |
| 35         | DA           | 1053       | C           |
| 35         | DA           | 1054       | A           |
| 35         | DA           | 1058       | G           |
| 35         | DA           | 1062       | G           |
| 35         | DA           | 1067       | A           |
| 35         | DA           | 1070       | A           |
| 35         | DA           | 1073       | A           |
| 35         | DA           | 1076       | C           |
| 35         | DA           | 1088       | A           |
| 35         | DA           | 1090       | U           |
| 35         | DA           | 1109       | C           |
| 35         | DA           | 1111       | A           |
| 35         | DA           | 1112       | G           |
| 35         | DA           | 1114       | G           |
| 35         | DA           | 1115       | G           |
| 35         | DA           | 1122       | G           |
| 35         | DA           | 1126       | A           |
| 35         | DA           | 1135       | C           |
| 35         | DA           | 1136       | G           |
| 35         | DA           | 1141       | U           |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | DA           | 1142       | U           |
| 35         | DA           | 1142(A)    | A           |
| 35         | DA           | 1143       | A           |
| 35         | DA           | 1146       | C           |
| 35         | DA           | 1155       | A           |
| 35         | DA           | 1157       | G           |
| 35         | DA           | 1158       | C           |
| 35         | DA           | 1159       | U           |
| 35         | DA           | 1170       | G           |
| 35         | DA           | 1173       | G           |
| 35         | DA           | 1174       | A           |
| 35         | DA           | 1175       | U           |
| 35         | DA           | 1176       | G           |
| 35         | DA           | 1177       | A           |
| 35         | DA           | 1204       | A           |
| 35         | DA           | 1210       | A           |
| 35         | DA           | 1211       | U           |
| 35         | DA           | 1212       | G           |
| 35         | DA           | 1213       | A           |
| 35         | DA           | 1220       | A           |
| 35         | DA           | 1221       | C           |
| 35         | DA           | 1224       | C           |
| 35         | DA           | 1238       | G           |
| 35         | DA           | 1247       | A           |
| 35         | DA           | 1248       | G           |
| 35         | DA           | 1250       | G           |
| 35         | DA           | 1251       | C           |
| 35         | DA           | 1252       | G           |
| 35         | DA           | 1255       | U           |
| 35         | DA           | 1256       | G           |
| 35         | DA           | 1266       | G           |
| 35         | DA           | 1271       | G           |
| 35         | DA           | 1272       | A           |
| 35         | DA           | 1273       | U           |
| 35         | DA           | 1287       | A           |
| 35         | DA           | 1300       | U           |
| 35         | DA           | 1302       | A           |
| 35         | DA           | 1314       | C           |
| 35         | DA           | 1326       | U           |
| 35         | DA           | 1329       | U           |
| 35         | DA           | 1330       | C           |
| 35         | DA           | 1332       | G           |

*Continued on next page...*



*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | DA           | 1342       | A           |
| 35         | DA           | 1345       | C           |
| 35         | DA           | 1349       | A           |
| 35         | DA           | 1359       | A           |
| 35         | DA           | 1365       | A           |
| 35         | DA           | 1379       | A           |
| 35         | DA           | 1380       | G           |
| 35         | DA           | 1384       | A           |
| 35         | DA           | 1385       | G           |
| 35         | DA           | 1386       | C           |
| 35         | DA           | 1396       | U           |
| 35         | DA           | 1403       | C           |
| 35         | DA           | 1406       | U           |
| 35         | DA           | 1411       | C           |
| 35         | DA           | 1416       | G           |
| 35         | DA           | 1420       | U           |
| 35         | DA           | 1421       | G           |
| 35         | DA           | 1427       | A           |
| 35         | DA           | 1428       | C           |
| 35         | DA           | 1434       | A           |
| 35         | DA           | 1435       | G           |
| 35         | DA           | 1445       | A           |
| 35         | DA           | 1445(A)    | C           |
| 35         | DA           | 1453       | U           |
| 35         | DA           | 1455       | G           |
| 35         | DA           | 1459       | G           |
| 35         | DA           | 1460       | A           |
| 35         | DA           | 1461       | G           |
| 35         | DA           | 1467       | C           |
| 35         | DA           | 1476       | C           |
| 35         | DA           | 1477       | A           |
| 35         | DA           | 1478       | G           |
| 35         | DA           | 1482       | G           |
| 35         | DA           | 1484       | G           |
| 35         | DA           | 1485       | G           |
| 35         | DA           | 1488       | G           |
| 35         | DA           | 1490       | A           |
| 35         | DA           | 1491       | G           |
| 35         | DA           | 1493       | C           |
| 35         | DA           | 1494       | A           |
| 35         | DA           | 1495       | A           |
| 35         | DA           | 1496       | A           |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 35  | DA    | 1497    | U    |
| 35  | DA    | 1505    | C    |
| 35  | DA    | 1509    | C    |
| 35  | DA    | 1509(A) | A    |
| 35  | DA    | 1517    | G    |
| 35  | DA    | 1528(A) | A    |
| 35  | DA    | 1541    | G    |
| 35  | DA    | 1542    | A    |
| 35  | DA    | 1544    | A    |
| 35  | DA    | 1553    | A    |
| 35  | DA    | 1554    | A    |
| 35  | DA    | 1559    | G    |
| 35  | DA    | 1569    | A    |
| 35  | DA    | 1578    | U    |
| 35  | DA    | 1579    | A    |
| 35  | DA    | 1584    | C    |
| 35  | DA    | 1586    | A    |
| 35  | DA    | 1588    | C    |
| 35  | DA    | 1603    | A    |
| 35  | DA    | 1608    | A    |
| 35  | DA    | 1609    | A    |
| 35  | DA    | 1610    | A    |
| 35  | DA    | 1615    | C    |
| 35  | DA    | 1616    | A    |
| 35  | DA    | 1618    | A    |
| 35  | DA    | 1634    | A    |
| 35  | DA    | 1640    | C    |
| 35  | DA    | 1644    | C    |
| 35  | DA    | 1648    | C    |
| 35  | DA    | 1668    | A    |
| 35  | DA    | 1674    | G    |
| 35  | DA    | 1678    | G    |
| 35  | DA    | 1698    | A    |
| 35  | DA    | 1699    | G    |
| 35  | DA    | 1718    | G    |
| 35  | DA    | 1722    | A    |
| 35  | DA    | 1739    | U    |
| 35  | DA    | 1740    | G    |
| 35  | DA    | 1744    | C    |
| 35  | DA    | 1748    | G    |
| 35  | DA    | 1763    | G    |
| 35  | DA    | 1764    | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 35  | DA    | 1773 | A    |
| 35  | DA    | 1780 | A    |
| 35  | DA    | 1781 | C    |
| 35  | DA    | 1784 | A    |
| 35  | DA    | 1787 | A    |
| 35  | DA    | 1791 | A    |
| 35  | DA    | 1799 | G    |
| 35  | DA    | 1800 | C    |
| 35  | DA    | 1801 | G    |
| 35  | DA    | 1815 | A    |
| 35  | DA    | 1816 | G    |
| 35  | DA    | 1820 | U    |
| 35  | DA    | 1821 | A    |
| 35  | DA    | 1829 | A    |
| 35  | DA    | 1839 | G    |
| 35  | DA    | 1846 | G    |
| 35  | DA    | 1847 | A    |
| 35  | DA    | 1850 | G    |
| 35  | DA    | 1858 | G    |
| 35  | DA    | 1862 | G    |
| 35  | DA    | 1866 | C    |
| 35  | DA    | 1878 | G    |
| 35  | DA    | 1885 | A    |
| 35  | DA    | 1888 | G    |
| 35  | DA    | 1889 | A    |
| 35  | DA    | 1900 | A    |
| 35  | DA    | 1906 | G    |
| 35  | DA    | 1912 | A    |
| 35  | DA    | 1929 | G    |
| 35  | DA    | 1930 | G    |
| 35  | DA    | 1931 | U    |
| 35  | DA    | 1937 | A    |
| 35  | DA    | 1938 | A    |
| 35  | DA    | 1943 | U    |
| 35  | DA    | 1944 | U    |
| 35  | DA    | 1945 | G    |
| 35  | DA    | 1948 | G    |
| 35  | DA    | 1955 | U    |
| 35  | DA    | 1960 | A    |
| 35  | DA    | 1963 | U    |
| 35  | DA    | 1964 | G    |
| 35  | DA    | 1967 | C    |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | DA           | 1969       | A           |
| 35         | DA           | 1970       | A           |
| 35         | DA           | 1971       | A           |
| 35         | DA           | 1972       | A           |
| 35         | DA           | 1993       | U           |
| 35         | DA           | 1997       | G           |
| 35         | DA           | 2004       | G           |
| 35         | DA           | 2021       | C           |
| 35         | DA           | 2022       | U           |
| 35         | DA           | 2023       | G           |
| 35         | DA           | 2031       | A           |
| 35         | DA           | 2033       | A           |
| 35         | DA           | 2034       | U           |
| 35         | DA           | 2043       | C           |
| 35         | DA           | 2055       | C           |
| 35         | DA           | 2056       | G           |
| 35         | DA           | 2060       | A           |
| 35         | DA           | 2061       | G           |
| 35         | DA           | 2062       | A           |
| 35         | DA           | 2065       | C           |
| 35         | DA           | 2069       | G           |
| 35         | DA           | 2076       | U           |
| 35         | DA           | 2100       | G           |
| 35         | DA           | 2103       | C           |
| 35         | DA           | 2104       | G           |
| 35         | DA           | 2112       | G           |
| 35         | DA           | 2116       | G           |
| 35         | DA           | 2118       | U           |
| 35         | DA           | 2127       | G           |
| 35         | DA           | 2132       | U           |
| 35         | DA           | 2133       | G           |
| 35         | DA           | 2134       | A           |
| 35         | DA           | 2157       | G           |
| 35         | DA           | 2158       | A           |
| 35         | DA           | 2159       | G           |
| 35         | DA           | 2163       | C           |
| 35         | DA           | 2172       | U           |
| 35         | DA           | 2173       | A           |
| 35         | DA           | 2185       | C           |
| 35         | DA           | 2187       | G           |
| 35         | DA           | 2189       | U           |
| 35         | DA           | 2190       | G           |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | DA           | 2192       | G           |
| 35         | DA           | 2193       | G           |
| 35         | DA           | 2198       | A           |
| 35         | DA           | 2199       | A           |
| 35         | DA           | 2200       | C           |
| 35         | DA           | 2202       | C           |
| 35         | DA           | 2203       | U           |
| 35         | DA           | 2205       | C           |
| 35         | DA           | 2206       | G           |
| 35         | DA           | 2207       | G           |
| 35         | DA           | 2208       | A           |
| 35         | DA           | 2219       | G           |
| 35         | DA           | 2225       | A           |
| 35         | DA           | 2226       | C           |
| 35         | DA           | 2238       | G           |
| 35         | DA           | 2239       | G           |
| 35         | DA           | 2263       | C           |
| 35         | DA           | 2273       | A           |
| 35         | DA           | 2283       | C           |
| 35         | DA           | 2286       | A           |
| 35         | DA           | 2288       | A           |
| 35         | DA           | 2297       | C           |
| 35         | DA           | 2302       | G           |
| 35         | DA           | 2305       | A           |
| 35         | DA           | 2306       | C           |
| 35         | DA           | 2307       | G           |
| 35         | DA           | 2308       | G           |
| 35         | DA           | 2309       | A           |
| 35         | DA           | 2313       | C           |
| 35         | DA           | 2319       | G           |
| 35         | DA           | 2320       | A           |
| 35         | DA           | 2325       | G           |
| 35         | DA           | 2334       | G           |
| 35         | DA           | 2336       | A           |
| 35         | DA           | 2345       | G           |
| 35         | DA           | 2346       | A           |
| 35         | DA           | 2347       | C           |
| 35         | DA           | 2348       | U           |
| 35         | DA           | 2349       | G           |
| 35         | DA           | 2350       | C           |
| 35         | DA           | 2383       | G           |
| 35         | DA           | 2385       | C           |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | DA           | 2402       | C           |
| 35         | DA           | 2423       | U           |
| 35         | DA           | 2424       | C           |
| 35         | DA           | 2425       | A           |
| 35         | DA           | 2427       | C           |
| 35         | DA           | 2428       | G           |
| 35         | DA           | 2429       | G           |
| 35         | DA           | 2430       | A           |
| 35         | DA           | 2431       | U           |
| 35         | DA           | 2434       | A           |
| 35         | DA           | 2435       | A           |
| 35         | DA           | 2439       | A           |
| 35         | DA           | 2441       | C           |
| 35         | DA           | 2448       | A           |
| 35         | DA           | 2461       | C           |
| 35         | DA           | 2465       | C           |
| 35         | DA           | 2469       | A           |
| 35         | DA           | 2470       | G           |
| 35         | DA           | 2473       | U           |
| 35         | DA           | 2474       | C           |
| 35         | DA           | 2475       | C           |
| 35         | DA           | 2476       | A           |
| 35         | DA           | 2477       | C           |
| 35         | DA           | 2478       | A           |
| 35         | DA           | 2482       | G           |
| 35         | DA           | 2484       | G           |
| 35         | DA           | 2502       | G           |
| 35         | DA           | 2503       | A           |
| 35         | DA           | 2505       | G           |
| 35         | DA           | 2519       | U           |
| 35         | DA           | 2520       | C           |
| 35         | DA           | 2524       | G           |
| 35         | DA           | 2529       | G           |
| 35         | DA           | 2543       | G           |
| 35         | DA           | 2554       | U           |
| 35         | DA           | 2566       | A           |
| 35         | DA           | 2567       | G           |
| 35         | DA           | 2572       | A           |
| 35         | DA           | 2573       | C           |
| 35         | DA           | 2577       | A           |
| 35         | DA           | 2585       | U           |
| 35         | DA           | 2586       | C           |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 35  | DA    | 2602    | A    |
| 35  | DA    | 2609    | U    |
| 35  | DA    | 2610    | C    |
| 35  | DA    | 2611    | U    |
| 35  | DA    | 2612    | C    |
| 35  | DA    | 2615    | U    |
| 35  | DA    | 2630    | G    |
| 35  | DA    | 2646    | C    |
| 35  | DA    | 2655    | G    |
| 35  | DA    | 2657    | A    |
| 35  | DA    | 2658    | C    |
| 35  | DA    | 2670    | A    |
| 35  | DA    | 2673    | G    |
| 35  | DA    | 2682    | U    |
| 35  | DA    | 2690    | C    |
| 35  | DA    | 2691    | C    |
| 35  | DA    | 2702    | U    |
| 35  | DA    | 2703    | C    |
| 35  | DA    | 2712    | U    |
| 35  | DA    | 2712(A) | A    |
| 35  | DA    | 2713    | A    |
| 35  | DA    | 2726    | U    |
| 35  | DA    | 2733    | A    |
| 35  | DA    | 2750    | A    |
| 35  | DA    | 2751    | G    |
| 35  | DA    | 2755    | C    |
| 35  | DA    | 2756    | U    |
| 35  | DA    | 2757    | A    |
| 35  | DA    | 2758    | A    |
| 35  | DA    | 2762    | G    |
| 35  | DA    | 2764    | A    |
| 35  | DA    | 2765    | A    |
| 35  | DA    | 2766    | G    |
| 35  | DA    | 2778    | A    |
| 35  | DA    | 2779    | U    |
| 35  | DA    | 2780    | G    |
| 35  | DA    | 2790    | A    |
| 35  | DA    | 2791    | C    |
| 35  | DA    | 2796    | U    |
| 35  | DA    | 2799    | C    |
| 35  | DA    | 2801    | A    |
| 35  | DA    | 2802    | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 35  | DA    | 2803 | C    |
| 35  | DA    | 2808 | U    |
| 35  | DA    | 2820 | A    |
| 35  | DA    | 2821 | A    |
| 35  | DA    | 2824 | C    |
| 35  | DA    | 2833 | G    |
| 35  | DA    | 2834 | G    |
| 35  | DA    | 2836 | U    |
| 35  | DA    | 2849 | U    |
| 35  | DA    | 2872 | G    |
| 35  | DA    | 2879 | C    |
| 35  | DA    | 2880 | C    |
| 35  | DA    | 2892 | A    |
| 35  | DA    | 2894 | G    |
| 35  | DA    | 2895 | U    |
| 36  | DB    | 8    | U    |
| 36  | DB    | 13   | A    |
| 36  | DB    | 15   | A    |
| 36  | DB    | 16   | G    |
| 36  | DB    | 22   | U    |
| 36  | DB    | 25   | A    |
| 36  | DB    | 33   | G    |
| 36  | DB    | 35   | U    |
| 36  | DB    | 41   | U    |
| 36  | DB    | 42   | C    |
| 36  | DB    | 45   | A    |
| 36  | DB    | 52   | A    |
| 36  | DB    | 53   | A    |
| 36  | DB    | 56   | G    |
| 36  | DB    | 67   | G    |
| 36  | DB    | 73   | A    |
| 36  | DB    | 81   | G    |
| 36  | DB    | 82   | G    |
| 36  | DB    | 88   | C    |
| 36  | DB    | 89   | G    |
| 36  | DB    | 90   | A    |
| 36  | DB    | 103  | G    |
| 36  | DB    | 104  | U    |
| 36  | DB    | 110  | G    |
| 36  | DB    | 113  | G    |

All (232) RNA pucker outliers are listed below:



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AA    | 30   | U    |
| 1   | AA    | 60   | A    |
| 1   | AA    | 115  | G    |
| 1   | AA    | 119  | A    |
| 1   | AA    | 203  | U    |
| 1   | AA    | 243  | A    |
| 1   | AA    | 250  | A    |
| 1   | AA    | 266  | G    |
| 1   | AA    | 315  | A    |
| 1   | AA    | 328  | C    |
| 1   | AA    | 344  | A    |
| 1   | AA    | 353  | A    |
| 1   | AA    | 366  | C    |
| 1   | AA    | 428  | G    |
| 1   | AA    | 429  | U    |
| 1   | AA    | 438  | G    |
| 1   | AA    | 532  | A    |
| 1   | AA    | 533  | A    |
| 1   | AA    | 535  | A    |
| 1   | AA    | 560  | U    |
| 1   | AA    | 575  | G    |
| 1   | AA    | 576  | G    |
| 1   | AA    | 631  | G    |
| 1   | AA    | 703  | G    |
| 1   | AA    | 812  | C    |
| 1   | AA    | 913  | A    |
| 1   | AA    | 992  | U    |
| 1   | AA    | 1049 | U    |
| 1   | AA    | 1065 | U    |
| 1   | AA    | 1101 | A    |
| 1   | AA    | 1129 | C    |
| 1   | AA    | 1201 | A    |
| 1   | AA    | 1225 | A    |
| 1   | AA    | 1226 | C    |
| 1   | AA    | 1285 | A    |
| 1   | AA    | 1299 | A    |
| 1   | AA    | 1300 | G    |
| 1   | AA    | 1337 | G    |
| 1   | AA    | 1347 | G    |
| 1   | AA    | 1364 | U    |
| 1   | AA    | 1493 | A    |
| 1   | AA    | 1498 | U    |
| 1   | AA    | 1505 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 22  | AW    | 73     | A    |
| 23  | AX    | 11     | U    |
| 35  | BA    | 27     | G    |
| 35  | BA    | 49     | A    |
| 35  | BA    | 74     | A    |
| 35  | BA    | 120    | U    |
| 35  | BA    | 128    | C    |
| 35  | BA    | 221    | A    |
| 35  | BA    | 226    | G    |
| 35  | BA    | 329    | G    |
| 35  | BA    | 331    | A    |
| 35  | BA    | 332    | A    |
| 35  | BA    | 363(F) | A    |
| 35  | BA    | 474    | G    |
| 35  | BA    | 503    | A    |
| 35  | BA    | 603    | A    |
| 35  | BA    | 614(A) | U    |
| 35  | BA    | 614(C) | A    |
| 35  | BA    | 728    | G    |
| 35  | BA    | 739    | G    |
| 35  | BA    | 752    | A    |
| 35  | BA    | 764    | A    |
| 35  | BA    | 961    | C    |
| 35  | BA    | 1020   | A    |
| 35  | BA    | 1022   | G    |
| 35  | BA    | 1052   | C    |
| 35  | BA    | 1057   | A    |
| 35  | BA    | 1156   | A    |
| 35  | BA    | 1173   | G    |
| 35  | BA    | 1210   | A    |
| 35  | BA    | 1212   | G    |
| 35  | BA    | 1237   | A    |
| 35  | BA    | 1301   | A    |
| 35  | BA    | 1378   | A    |
| 35  | BA    | 1427   | A    |
| 35  | BA    | 1453   | U    |
| 35  | BA    | 1494   | A    |
| 35  | BA    | 1541   | G    |
| 35  | BA    | 1558   | A    |
| 35  | BA    | 1799   | G    |
| 35  | BA    | 1819   | A    |
| 35  | BA    | 1838   | C    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 35  | BA    | 1846    | G    |
| 35  | BA    | 1930    | G    |
| 35  | BA    | 1943    | U    |
| 35  | BA    | 1948    | G    |
| 35  | BA    | 1992    | G    |
| 35  | BA    | 2033    | A    |
| 35  | BA    | 2111    | C    |
| 35  | BA    | 2126    | A    |
| 35  | BA    | 2172    | U    |
| 35  | BA    | 2198    | A    |
| 35  | BA    | 2225    | A    |
| 35  | BA    | 2282    | G    |
| 35  | BA    | 2296    | U    |
| 35  | BA    | 2344    | U    |
| 35  | BA    | 2345    | G    |
| 35  | BA    | 2422    | A    |
| 35  | BA    | 2425    | A    |
| 35  | BA    | 2428    | G    |
| 35  | BA    | 2481    | G    |
| 35  | BA    | 2611    | U    |
| 35  | BA    | 2689    | U    |
| 35  | BA    | 2690    | C    |
| 35  | BA    | 2756    | U    |
| 35  | BA    | 2762    | G    |
| 35  | BA    | 2778    | A    |
| 35  | BA    | 2779    | U    |
| 35  | BA    | 2799    | C    |
| 35  | BA    | 2801(A) | A    |
| 35  | BA    | 2835    | A    |
| 35  | BA    | 2849    | U    |
| 35  | BA    | 2891    | G    |
| 1   | CA    | 30      | U    |
| 1   | CA    | 60      | A    |
| 1   | CA    | 115     | G    |
| 1   | CA    | 119     | A    |
| 1   | CA    | 203     | U    |
| 1   | CA    | 243     | A    |
| 1   | CA    | 250     | A    |
| 1   | CA    | 266     | G    |
| 1   | CA    | 315     | A    |
| 1   | CA    | 328     | C    |
| 1   | CA    | 344     | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | CA    | 353  | A    |
| 1   | CA    | 366  | C    |
| 1   | CA    | 428  | G    |
| 1   | CA    | 429  | U    |
| 1   | CA    | 438  | G    |
| 1   | CA    | 532  | A    |
| 1   | CA    | 533  | A    |
| 1   | CA    | 534  | U    |
| 1   | CA    | 535  | A    |
| 1   | CA    | 560  | U    |
| 1   | CA    | 575  | G    |
| 1   | CA    | 576  | G    |
| 1   | CA    | 631  | G    |
| 1   | CA    | 703  | G    |
| 1   | CA    | 812  | C    |
| 1   | CA    | 913  | A    |
| 1   | CA    | 992  | U    |
| 1   | CA    | 1049 | U    |
| 1   | CA    | 1065 | U    |
| 1   | CA    | 1101 | A    |
| 1   | CA    | 1129 | C    |
| 1   | CA    | 1201 | A    |
| 1   | CA    | 1225 | A    |
| 1   | CA    | 1226 | C    |
| 1   | CA    | 1285 | A    |
| 1   | CA    | 1299 | A    |
| 1   | CA    | 1300 | G    |
| 1   | CA    | 1337 | G    |
| 1   | CA    | 1347 | G    |
| 1   | CA    | 1364 | U    |
| 1   | CA    | 1493 | A    |
| 1   | CA    | 1498 | U    |
| 22  | CW    | 73   | A    |
| 23  | CX    | 11   | U    |
| 35  | DA    | 27   | G    |
| 35  | DA    | 49   | A    |
| 35  | DA    | 74   | A    |
| 35  | DA    | 120  | U    |
| 35  | DA    | 128  | C    |
| 35  | DA    | 221  | A    |
| 35  | DA    | 226  | G    |
| 35  | DA    | 329  | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 35  | DA    | 331    | A    |
| 35  | DA    | 332    | A    |
| 35  | DA    | 363(F) | A    |
| 35  | DA    | 474    | G    |
| 35  | DA    | 503    | A    |
| 35  | DA    | 603    | A    |
| 35  | DA    | 614(A) | U    |
| 35  | DA    | 614(C) | A    |
| 35  | DA    | 728    | G    |
| 35  | DA    | 739    | G    |
| 35  | DA    | 752    | A    |
| 35  | DA    | 764    | A    |
| 35  | DA    | 961    | C    |
| 35  | DA    | 1020   | A    |
| 35  | DA    | 1022   | G    |
| 35  | DA    | 1052   | C    |
| 35  | DA    | 1057   | A    |
| 35  | DA    | 1156   | A    |
| 35  | DA    | 1173   | G    |
| 35  | DA    | 1210   | A    |
| 35  | DA    | 1212   | G    |
| 35  | DA    | 1237   | A    |
| 35  | DA    | 1301   | A    |
| 35  | DA    | 1378   | A    |
| 35  | DA    | 1427   | A    |
| 35  | DA    | 1453   | U    |
| 35  | DA    | 1494   | A    |
| 35  | DA    | 1541   | G    |
| 35  | DA    | 1558   | A    |
| 35  | DA    | 1799   | G    |
| 35  | DA    | 1819   | A    |
| 35  | DA    | 1838   | C    |
| 35  | DA    | 1846   | G    |
| 35  | DA    | 1930   | G    |
| 35  | DA    | 1943   | U    |
| 35  | DA    | 1948   | G    |
| 35  | DA    | 1992   | G    |
| 35  | DA    | 2033   | A    |
| 35  | DA    | 2111   | C    |
| 35  | DA    | 2126   | A    |
| 35  | DA    | 2172   | U    |
| 35  | DA    | 2198   | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 35  | DA    | 2225    | A    |
| 35  | DA    | 2282    | G    |
| 35  | DA    | 2296    | U    |
| 35  | DA    | 2344    | U    |
| 35  | DA    | 2345    | G    |
| 35  | DA    | 2422    | A    |
| 35  | DA    | 2425    | A    |
| 35  | DA    | 2428    | G    |
| 35  | DA    | 2481    | G    |
| 35  | DA    | 2611    | U    |
| 35  | DA    | 2689    | U    |
| 35  | DA    | 2690    | C    |
| 35  | DA    | 2756    | U    |
| 35  | DA    | 2762    | G    |
| 35  | DA    | 2778    | A    |
| 35  | DA    | 2779    | U    |
| 35  | DA    | 2799    | C    |
| 35  | DA    | 2801(A) | A    |
| 35  | DA    | 2835    | A    |
| 35  | DA    | 2849    | U    |
| 35  | DA    | 2891    | G    |

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 22  | 5MU  | AV    | 54  | 22   | 14,21,23     | 1.21 | 2 (14%)     | 15,30,35    | 4.07 | 2 (13%)     |
| 22  | 5MU  | AW    | 55  | 22   | 14,21,23     | 1.19 | 2 (14%)     | 15,30,35    | 4.13 | 2 (13%)     |
| 22  | 5MU  | CV    | 54  | 22   | 14,21,23     | 1.14 | 2 (14%)     | 15,30,35    | 4.10 | 2 (13%)     |
| 22  | 5MU  | CW    | 55  | 22   | 14,21,23     | 1.19 | 2 (14%)     | 15,30,35    | 4.09 | 2 (13%)     |

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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 22  | 5MU  | AV    | 54  | 22   | -       | 0/3/25/26 | 0/2/2/2 |
| 22  | 5MU  | AW    | 55  | 22   | -       | 0/3/25/26 | 0/2/2/2 |
| 22  | 5MU  | CV    | 54  | 22   | -       | 0/3/25/26 | 0/2/2/2 |
| 22  | 5MU  | CW    | 55  | 22   | -       | 0/3/25/26 | 0/2/2/2 |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 22  | CW    | 55  | 5MU  | C6-N1 | 2.06 | 1.38        | 1.35     |
| 22  | CV    | 54  | 5MU  | C6-N1 | 2.08 | 1.38        | 1.35     |
| 22  | AW    | 55  | 5MU  | C6-N1 | 2.09 | 1.38        | 1.35     |
| 22  | AV    | 54  | 5MU  | C6-N1 | 2.11 | 1.38        | 1.35     |
| 22  | CV    | 54  | 5MU  | C4-N3 | 3.12 | 1.38        | 1.33     |
| 22  | AV    | 54  | 5MU  | C4-N3 | 3.20 | 1.38        | 1.33     |
| 22  | CW    | 55  | 5MU  | C4-N3 | 3.24 | 1.38        | 1.33     |
| 22  | AW    | 55  | 5MU  | C4-N3 | 3.33 | 1.39        | 1.33     |

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 22  | AW    | 55  | 5MU  | C5-C4-N3 | -3.32 | 115.19      | 123.12   |
| 22  | CV    | 54  | 5MU  | C5-C4-N3 | -3.32 | 115.20      | 123.12   |
| 22  | CW    | 55  | 5MU  | C5-C4-N3 | -3.30 | 115.23      | 123.12   |
| 22  | AV    | 54  | 5MU  | C5-C4-N3 | -3.18 | 115.52      | 123.12   |
| 22  | AV    | 54  | 5MU  | C4-N3-C2 | 15.32 | 127.29      | 114.13   |
| 22  | CW    | 55  | 5MU  | C4-N3-C2 | 15.37 | 127.34      | 114.13   |
| 22  | CV    | 54  | 5MU  | C4-N3-C2 | 15.40 | 127.36      | 114.13   |
| 22  | AW    | 55  | 5MU  | C4-N3-C2 | 15.50 | 127.44      | 114.13   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 22  | AV    | 54  | 5MU  | 2       | 0            |
| 22  | AW    | 55  | 5MU  | 1       | 0            |
| 22  | CV    | 54  | 5MU  | 1       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 22  | CW    | 55  | 5MU  | 2       | 0            |

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 61  | FUA  | AY    | 702 | -    | 37,40,40     | 1.71 | 6 (16%)  | 45,64,64    | 1.72 | 7 (15%)  |
| 62  | GDP  | AY    | 703 | 60   | 25,30,30     | 1.28 | 3 (12%)  | 26,47,47    | 2.03 | 6 (23%)  |
| 61  | FUA  | CY    | 702 | -    | 37,40,40     | 1.72 | 6 (16%)  | 45,64,64    | 1.57 | 9 (20%)  |
| 62  | GDP  | CY    | 703 | 60   | 25,30,30     | 1.32 | 3 (12%)  | 26,47,47    | 2.25 | 8 (30%)  |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 61  | FUA  | AY    | 702 | -    | -       | 0/10/92/92 | 0/4/4/4 |
| 62  | GDP  | AY    | 703 | 60   | -       | 0/12/32/32 | 0/3/3/3 |
| 61  | FUA  | CY    | 702 | -    | -       | 0/10/92/92 | 0/4/4/4 |
| 62  | GDP  | CY    | 703 | 60   | -       | 0/12/32/32 | 0/3/3/3 |

All (18) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 61  | CY    | 702 | FUA  | C23-C22 | -6.57 | 1.39        | 1.51     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 61  | AY    | 702 | FUA  | C23-C22 | -6.39 | 1.39        | 1.51     |
| 61  | AY    | 702 | FUA  | C23-C24 | -4.14 | 1.39        | 1.53     |
| 61  | CY    | 702 | FUA  | C23-C24 | -4.14 | 1.39        | 1.53     |
| 61  | CY    | 702 | FUA  | C24-C25 | -3.25 | 1.39        | 1.50     |
| 61  | AY    | 702 | FUA  | C24-C25 | -3.14 | 1.39        | 1.50     |
| 61  | AY    | 702 | FUA  | C14-C8  | -2.88 | 1.53        | 1.58     |
| 61  | CY    | 702 | FUA  | C14-C8  | -2.86 | 1.53        | 1.58     |
| 61  | CY    | 702 | FUA  | C10-C9  | -2.15 | 1.53        | 1.57     |
| 61  | AY    | 702 | FUA  | C10-C9  | -2.11 | 1.53        | 1.57     |
| 62  | AY    | 703 | GDP  | O4'-C1' | 2.10  | 1.44        | 1.41     |
| 61  | AY    | 702 | FUA  | C25-C26 | 2.35  | 1.39        | 1.32     |
| 62  | CY    | 703 | GDP  | O4'-C1' | 2.42  | 1.44        | 1.41     |
| 61  | CY    | 702 | FUA  | C25-C26 | 2.53  | 1.39        | 1.32     |
| 62  | CY    | 703 | GDP  | C2-N1   | 2.77  | 1.40        | 1.35     |
| 62  | AY    | 703 | GDP  | C2-N1   | 2.95  | 1.40        | 1.35     |
| 62  | AY    | 703 | GDP  | C6-N1   | 3.94  | 1.40        | 1.33     |
| 62  | CY    | 703 | GDP  | C6-N1   | 4.28  | 1.40        | 1.33     |

All (30) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 62  | CY    | 703 | GDP  | N3-C2-N1    | -5.00 | 120.16      | 127.46   |
| 62  | AY    | 703 | GDP  | N3-C2-N1    | -4.99 | 120.17      | 127.46   |
| 61  | AY    | 702 | FUA  | C13-C12-C11 | -4.41 | 105.84      | 111.97   |
| 61  | CY    | 702 | FUA  | C16-O2-C31  | -4.15 | 110.67      | 117.10   |
| 62  | CY    | 703 | GDP  | C4'-O4'-C1' | -3.90 | 105.62      | 109.77   |
| 61  | AY    | 702 | FUA  | C16-O2-C31  | -3.86 | 111.12      | 117.10   |
| 62  | AY    | 703 | GDP  | C4'-O4'-C1' | -3.62 | 105.92      | 109.77   |
| 62  | CY    | 703 | GDP  | C2'-C3'-C4' | -3.60 | 95.61       | 102.62   |
| 61  | AY    | 702 | FUA  | C8-C9-C10   | -3.49 | 112.82      | 116.44   |
| 62  | AY    | 703 | GDP  | C5-C6-N1    | -3.41 | 118.63      | 123.48   |
| 62  | CY    | 703 | GDP  | C5-C6-N1    | -3.30 | 118.78      | 123.48   |
| 61  | CY    | 702 | FUA  | C13-C12-C11 | -3.23 | 107.47      | 111.97   |
| 61  | CY    | 702 | FUA  | C8-C9-C10   | -2.93 | 113.40      | 116.44   |
| 62  | CY    | 703 | GDP  | C4-C5-N7    | -2.85 | 106.65      | 109.41   |
| 62  | AY    | 703 | GDP  | C4-C5-N7    | -2.44 | 107.05      | 109.41   |
| 61  | CY    | 702 | FUA  | C19-C10-C9  | -2.11 | 108.03      | 113.13   |
| 61  | CY    | 702 | FUA  | C24-C25-C26 | -2.08 | 120.39      | 127.80   |
| 61  | AY    | 702 | FUA  | C12-C13-C14 | -2.02 | 110.43      | 114.72   |
| 61  | CY    | 702 | FUA  | C23-C24-C25 | 2.16  | 119.39      | 111.97   |
| 61  | AY    | 702 | FUA  | C28-C26-C27 | 2.21  | 119.75      | 114.60   |
| 62  | CY    | 703 | GDP  | C6-N1-C2    | 2.22  | 119.25      | 116.06   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 62  | AY    | 703 | GDP  | C6-N1-C2    | 2.23 | 119.27      | 116.06   |
| 61  | CY    | 702 | FUA  | O2-C31-C32  | 2.23 | 115.29      | 111.10   |
| 62  | CY    | 703 | GDP  | N2-C2-N1    | 2.24 | 120.83      | 117.24   |
| 61  | CY    | 702 | FUA  | C28-C26-C27 | 2.29 | 119.93      | 114.60   |
| 61  | AY    | 702 | FUA  | O2-C31-C32  | 2.89 | 116.52      | 111.10   |
| 61  | CY    | 702 | FUA  | C24-C23-C22 | 3.92 | 121.43      | 112.50   |
| 61  | AY    | 702 | FUA  | C24-C23-C22 | 5.10 | 124.11      | 112.50   |
| 62  | AY    | 703 | GDP  | C2-N3-C4    | 5.41 | 121.48      | 115.16   |
| 62  | CY    | 703 | GDP  | C2-N3-C4    | 5.67 | 121.78      | 115.16   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 51 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 61  | AY    | 702 | FUA  | 13      | 0            |
| 62  | AY    | 703 | GDP  | 8       | 0            |
| 61  | CY    | 702 | FUA  | 22      | 0            |
| 62  | CY    | 703 | GDP  | 8       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 9   | AI    | 2                |
| 9   | CI    | 2                |
| 45  | BL    | 1                |
| 41  | DG    | 1                |
| 41  | BG    | 1                |
| 45  | DL    | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | DL    | 30:UNK    | C      | 52:UNK    | N      | 38.40        |
| 1     | BL    | 30:UNK    | C      | 52:UNK    | N      | 36.36        |
| 1     | BG    | 112:PRO   | C      | 113:ARG   | N      | 3.27         |
| 1     | DG    | 112:PRO   | C      | 113:ARG   | N      | 3.05         |
| 1     | CI    | 53:VAL    | C      | 54:ASP    | N      | 2.98         |
| 1     | AI    | 53:VAL    | C      | 54:ASP    | N      | 2.92         |
| 1     | AI    | 104:ARG   | C      | 105:ASP   | N      | 2.54         |
| 1     | CI    | 104:ARG   | C      | 105:ASP   | N      | 2.54         |

## 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    | 1504/1522 (98%) | -0.27  | 22 (1%) 74 61 | 23, 62, 148, 220      | 0     |
| 1   | CA    | 1504/1522 (98%) | -0.52  | 15 (0%) 82 70 | 26, 65, 148, 220      | 0     |
| 2   | AB    | 235/256 (91%)   | -0.31  | 3 (1%) 77 64  | 40, 81, 147, 159      | 0     |
| 2   | CB    | 235/256 (91%)   | -0.33  | 1 (0%) 92 87  | 43, 82, 147, 158      | 0     |
| 3   | AC    | 207/239 (86%)   | -0.41  | 0 100 100     | 31, 72, 113, 118      | 0     |
| 3   | CC    | 207/239 (86%)   | -0.38  | 0 100 100     | 33, 75, 115, 121      | 0     |
| 4   | AD    | 208/209 (99%)   | -0.39  | 0 100 100     | 47, 79, 115, 124      | 0     |
| 4   | CD    | 208/209 (99%)   | -0.43  | 0 100 100     | 48, 80, 116, 125      | 0     |
| 5   | AE    | 151/162 (93%)   | -0.49  | 1 (0%) 87 78  | 25, 50, 90, 112       | 0     |
| 5   | CE    | 151/162 (93%)   | -0.46  | 1 (0%) 87 78  | 27, 52, 91, 112       | 0     |
| 6   | AF    | 101/101 (100%)  | -0.44  | 0 100 100     | 55, 85, 110, 118      | 0     |
| 6   | CF    | 101/101 (100%)  | -0.29  | 0 100 100     | 60, 87, 111, 118      | 0     |
| 7   | AG    | 155/156 (99%)   | -0.39  | 1 (0%) 89 81  | 51, 79, 109, 136      | 0     |
| 7   | CG    | 155/156 (99%)   | -0.39  | 2 (1%) 77 64  | 55, 81, 111, 136      | 0     |
| 8   | AH    | 138/138 (100%)  | -0.41  | 0 100 100     | 32, 54, 75, 82        | 0     |
| 8   | CH    | 138/138 (100%)  | -0.49  | 0 100 100     | 35, 56, 76, 83        | 0     |
| 9   | AI    | 127/128 (99%)   | -0.23  | 1 (0%) 86 75  | 50, 83, 114, 120      | 0     |
| 9   | CI    | 127/128 (99%)   | -0.37  | 1 (0%) 86 75  | 53, 86, 114, 120      | 0     |
| 10  | AJ    | 99/105 (94%)    | 0.08   | 6 (6%) 22 16  | 47, 100, 155, 159     | 0     |
| 10  | CJ    | 99/105 (94%)    | 0.17   | 3 (3%) 51 37  | 50, 102, 156, 159     | 0     |
| 11  | AK    | 119/129 (92%)   | -0.34  | 2 (1%) 70 57  | 42, 59, 100, 123      | 0     |
| 11  | CK    | 119/129 (92%)   | -0.28  | 1 (0%) 86 75  | 44, 60, 102, 124      | 0     |
| 12  | AL    | 125/132 (94%)   | -0.49  | 0 100 100     | 38, 57, 87, 127       | 0     |
| 12  | CL    | 125/132 (94%)   | -0.44  | 2 (1%) 72 59  | 39, 58, 88, 129       | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|---------------|-----------------------|-------|
| 13  | AM    | 125/126 (99%) | -0.15  | 6 (4%) 31 22  | 68, 111, 139, 171     | 0     |
| 13  | CM    | 125/126 (99%) | -0.16  | 8 (6%) 20 14  | 70, 112, 139, 172     | 0     |
| 14  | AN    | 60/61 (98%)   | -0.41  | 1 (1%) 70 57  | 39, 59, 92, 97        | 0     |
| 14  | CN    | 60/61 (98%)   | -0.42  | 0 100 100     | 44, 61, 93, 98        | 0     |
| 15  | AO    | 88/89 (98%)   | -0.57  | 0 100 100     | 35, 61, 91, 100       | 0     |
| 15  | CO    | 88/89 (98%)   | -0.55  | 0 100 100     | 38, 61, 94, 100       | 0     |
| 16  | AP    | 84/88 (95%)   | -0.45  | 0 100 100     | 54, 73, 96, 131       | 0     |
| 16  | CP    | 84/88 (95%)   | -0.43  | 1 (1%) 79 66  | 57, 74, 98, 132       | 0     |
| 17  | AQ    | 100/105 (95%) | -0.56  | 0 100 100     | 43, 64, 89, 98        | 0     |
| 17  | CQ    | 100/105 (95%) | -0.50  | 0 100 100     | 46, 66, 90, 97        | 0     |
| 18  | AR    | 70/88 (79%)   | -0.42  | 1 (1%) 75 62  | 42, 69, 94, 108       | 0     |
| 18  | CR    | 70/88 (79%)   | -0.51  | 1 (1%) 75 62  | 45, 70, 95, 109       | 0     |
| 19  | AS    | 79/93 (84%)   | -0.02  | 2 (2%) 58 43  | 77, 106, 144, 149     | 0     |
| 19  | CS    | 79/93 (84%)   | 0.15   | 4 (5%) 29 20  | 78, 107, 144, 150     | 0     |
| 20  | AT    | 99/106 (93%)  | -0.37  | 0 100 100     | 63, 84, 126, 129      | 0     |
| 20  | CT    | 99/106 (93%)  | -0.37  | 0 100 100     | 64, 85, 127, 129      | 0     |
| 21  | AU    | 25/27 (92%)   | -0.24  | 0 100 100     | 63, 82, 118, 122      | 0     |
| 21  | CU    | 25/27 (92%)   | 0.12   | 0 100 100     | 66, 86, 120, 123      | 0     |
| 22  | AV    | 76/77 (98%)   | -0.49  | 0 100 100     | 32, 67, 110, 127      | 0     |
| 22  | AW    | 76/77 (98%)   | -0.43  | 1 (1%) 77 64  | 71, 168, 192, 201     | 0     |
| 22  | CV    | 76/77 (98%)   | -0.62  | 0 100 100     | 47, 84, 121, 151      | 0     |
| 22  | CW    | 76/77 (98%)   | -0.37  | 1 (1%) 77 64  | 78, 176, 200, 210     | 0     |
| 23  | AX    | 11/25 (44%)   | 0.08   | 0 100 100     | 28, 94, 149, 166      | 0     |
| 23  | CX    | 11/25 (44%)   | 0.00   | 0 100 100     | 45, 106, 156, 168     | 0     |
| 24  | AY    | 667/691 (96%) | -0.18  | 9 (1%) 77 64  | 61, 99, 140, 150      | 0     |
| 24  | CY    | 667/691 (96%) | 0.07   | 23 (3%) 46 33 | 73, 108, 148, 161     | 0     |
| 25  | B0    | 84/85 (98%)   | 0.04   | 6 (7%) 17 12  | 67, 82, 140, 163      | 0     |
| 25  | D0    | 84/85 (98%)   | 0.37   | 9 (10%) 7 6   | 69, 84, 141, 163      | 0     |
| 26  | B1    | 94/98 (95%)   | -0.46  | 1 (1%) 80 67  | 41, 70, 118, 128      | 0     |
| 26  | D1    | 94/98 (95%)   | -0.34  | 0 100 100     | 53, 80, 123, 131      | 0     |
| 27  | B2    | 71/72 (98%)   | -0.30  | 2 (2%) 53 40  | 77, 116, 150, 161     | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 27  | D2    | 71/72 (98%)     | -0.15  | 2 (2%) 53 40  | 95, 119, 146, 163     | 0     |
| 28  | B3    | 60/60 (100%)    | -0.09  | 1 (1%) 70 57  | 63, 88, 114, 135      | 0     |
| 28  | D3    | 60/60 (100%)    | -0.02  | 2 (3%) 47 35  | 64, 89, 114, 134      | 0     |
| 29  | B4    | 58/71 (81%)     | 0.07   | 3 (5%) 28 20  | 76, 135, 220, 222     | 0     |
| 29  | D4    | 58/71 (81%)     | 0.27   | 7 (12%) 5 5   | 77, 137, 220, 222     | 0     |
| 30  | B5    | 59/60 (98%)     | -0.08  | 3 (5%) 29 20  | 52, 80, 153, 172      | 0     |
| 30  | D5    | 59/60 (98%)     | -0.03  | 4 (6%) 18 13  | 52, 80, 153, 172      | 0     |
| 31  | B6    | 50/54 (92%)     | -0.00  | 2 (4%) 39 28  | 56, 89, 107, 117      | 0     |
| 31  | D6    | 50/54 (92%)     | -0.26  | 1 (2%) 65 51  | 56, 90, 108, 117      | 0     |
| 32  | B7    | 49/49 (100%)    | -0.34  | 2 (4%) 38 27  | 47, 64, 119, 132      | 0     |
| 32  | D7    | 49/49 (100%)    | -0.39  | 0 100 100     | 47, 64, 120, 132      | 0     |
| 33  | B8    | 64/65 (98%)     | -0.37  | 1 (1%) 72 59  | 63, 75, 105, 125      | 0     |
| 33  | D8    | 64/65 (98%)     | -0.26  | 1 (1%) 72 59  | 65, 76, 105, 126      | 0     |
| 34  | B9    | 37/37 (100%)    | -0.43  | 0 100 100     | 60, 71, 85, 89        | 0     |
| 34  | D9    | 37/37 (100%)    | -0.30  | 1 (2%) 55 41  | 60, 73, 87, 91        | 0     |
| 35  | BA    | 2901/2915 (99%) | -0.40  | 27 (0%) 84 72 | 30, 76, 162, 221      | 0     |
| 35  | DA    | 2901/2915 (99%) | -0.53  | 32 (1%) 80 67 | 29, 77, 162, 221      | 0     |
| 36  | BB    | 119/122 (97%)   | -0.54  | 0 100 100     | 65, 106, 138, 183     | 0     |
| 36  | DB    | 119/122 (97%)   | -0.72  | 0 100 100     | 66, 108, 138, 183     | 0     |
| 37  | BC    | 228/229 (99%)   | -0.13  | 4 (1%) 69 55  | 42, 97, 147, 160      | 0     |
| 37  | DC    | 228/229 (99%)   | 0.09   | 11 (4%) 31 22 | 43, 98, 148, 162      | 0     |
| 38  | BD    | 275/276 (99%)   | -0.52  | 0 100 100     | 31, 52, 82, 101       | 0     |
| 38  | DD    | 275/276 (99%)   | -0.51  | 1 (0%) 92 87  | 32, 52, 82, 101       | 0     |
| 39  | BE    | 205/206 (99%)   | -0.33  | 3 (1%) 74 61  | 44, 77, 128, 135      | 0     |
| 39  | DE    | 205/206 (99%)   | -0.29  | 3 (1%) 74 61  | 44, 77, 128, 134      | 0     |
| 40  | BF    | 208/210 (99%)   | 0.01   | 10 (4%) 31 22 | 53, 110, 166, 177     | 0     |
| 40  | DF    | 208/210 (99%)   | -0.01  | 12 (5%) 24 17 | 53, 111, 166, 176     | 0     |
| 41  | BG    | 181/182 (99%)   | -0.27  | 4 (2%) 62 48  | 63, 95, 131, 143      | 0     |
| 41  | DG    | 181/182 (99%)   | -0.03  | 6 (3%) 47 35  | 86, 110, 137, 151     | 0     |
| 42  | BH    | 167/180 (92%)   | 0.06   | 6 (3%) 43 32  | 81, 117, 143, 159     | 0     |
| 42  | DH    | 167/180 (92%)   | 0.04   | 4 (2%) 59 45  | 81, 118, 143, 160     | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 43  | BJ    | 0/173          | -      | -            | -                     | -     |
| 43  | DJ    | 0/173          | -      | -            | -                     | -     |
| 44  | BK    | 140/147 (95%)  | 1.96   | 61 (43%) 0 0 | 162, 180, 186, 188    | 0     |
| 44  | DK    | 140/147 (95%)  | 1.68   | 49 (35%) 0 1 | 162, 180, 186, 187    | 0     |
| 45  | BL    | 0/125          | -      | -            | -                     | -     |
| 45  | BM    | 0/125          | -      | -            | -                     | -     |
| 45  | Bl    | 0/125          | -      | -            | -                     | -     |
| 45  | Bm    | 0/125          | -      | -            | -                     | -     |
| 45  | DL    | 0/125          | -      | -            | -                     | -     |
| 45  | DM    | 0/125          | -      | -            | -                     | -     |
| 45  | Dl    | 0/125          | -      | -            | -                     | -     |
| 45  | Dm    | 0/125          | -      | -            | -                     | -     |
| 46  | BN    | 139/140 (99%)  | -0.30  | 2 (1%) 75 62 | 60, 91, 132, 137      | 0     |
| 46  | DN    | 139/140 (99%)  | -0.25  | 1 (0%) 87 78 | 61, 91, 132, 137      | 0     |
| 47  | BO    | 122/122 (100%) | -0.46  | 0 100 100    | 35, 60, 73, 86        | 0     |
| 47  | DO    | 122/122 (100%) | -0.44  | 0 100 100    | 36, 61, 73, 88        | 0     |
| 48  | BP    | 146/150 (97%)  | 0.02   | 4 (2%) 55 41 | 46, 111, 137, 157     | 0     |
| 48  | DP    | 146/150 (97%)  | 0.10   | 4 (2%) 55 41 | 50, 113, 137, 157     | 0     |
| 49  | BQ    | 141/141 (100%) | -0.38  | 0 100 100    | 45, 65, 88, 119       | 0     |
| 49  | DQ    | 141/141 (100%) | -0.41  | 0 100 100    | 45, 66, 89, 120       | 0     |
| 50  | BR    | 117/118 (99%)  | -0.37  | 1 (0%) 84 72 | 49, 81, 101, 128      | 0     |
| 50  | DR    | 117/118 (99%)  | -0.28  | 1 (0%) 84 72 | 53, 82, 101, 128      | 0     |
| 51  | BS    | 99/112 (88%)   | -0.19  | 2 (2%) 65 51 | 82, 116, 140, 144     | 0     |
| 51  | DS    | 99/112 (88%)   | 0.28   | 5 (5%) 29 20 | 83, 117, 141, 145     | 0     |
| 52  | BT    | 138/146 (94%)  | -0.13  | 4 (2%) 52 38 | 55, 83, 149, 176      | 0     |
| 52  | DT    | 138/146 (94%)  | -0.18  | 5 (3%) 43 32 | 57, 84, 149, 177      | 0     |
| 53  | BU    | 117/118 (99%)  | -0.37  | 0 100 100    | 62, 80, 114, 135      | 0     |
| 53  | DU    | 117/118 (99%)  | -0.36  | 0 100 100    | 62, 81, 115, 134      | 0     |
| 54  | BV    | 101/101 (100%) | -0.03  | 1 (0%) 82 70 | 59, 116, 133, 141     | 0     |
| 54  | DV    | 101/101 (100%) | 0.17   | 5 (4%) 30 21 | 61, 116, 134, 140     | 0     |
| 55  | BW    | 113/113 (100%) | -0.28  | 0 100 100    | 61, 79, 119, 158      | 0     |
| 55  | DW    | 113/113 (100%) | -0.16  | 0 100 100    | 63, 80, 120, 159      | 0     |
| 56  | BX    | 93/96 (96%)    | -0.18  | 0 100 100    | 76, 91, 110, 114      | 0     |
| 56  | DX    | 93/96 (96%)    | -0.22  | 0 100 100    | 76, 92, 111, 114      | 0     |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 57  | BY    | 107/110 (97%)     | 0.08   | 2 (1%) 67 53   | 78, 127, 149, 155     | 0     |
| 57  | DY    | 107/110 (97%)     | 0.41   | 4 (3%) 42 31   | 78, 127, 149, 155     | 0     |
| 58  | BZ    | 185/206 (89%)     | -0.23  | 1 (0%) 90 84   | 47, 90, 135, 143      | 0     |
| 58  | DZ    | 185/206 (89%)     | -0.09  | 1 (0%) 90 84   | 68, 99, 138, 146      | 0     |
| All | All   | 22794/24788 (91%) | -0.29  | 444 (1%) 67 53 | 23, 82, 155, 222      | 0     |

All (444) RSRZ outliers are listed below:

| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 35  | BA    | 654(K)  | C    | 14.8 |
| 1   | CA    | 1036    | G    | 13.4 |
| 52  | BT    | 138     | ALA  | 13.1 |
| 35  | DA    | 654(D)  | G    | 13.0 |
| 35  | BA    | 654(F)  | C    | 11.4 |
| 35  | BA    | 654(I)  | C    | 11.3 |
| 1   | AA    | 1026    | G    | 11.3 |
| 44  | BK    | 16      | LYS  | 10.9 |
| 1   | AA    | 1030(B) | C    | 10.1 |
| 1   | CA    | 89      | C    | 9.9  |
| 1   | AA    | 1036    | G    | 9.7  |
| 1   | AA    | 89      | C    | 9.6  |
| 41  | DG    | 49      | ASP  | 9.5  |
| 52  | DT    | 134     | GLU  | 9.3  |
| 35  | DA    | 654(J)  | A    | 9.3  |
| 35  | DA    | 654(E)  | G    | 9.2  |
| 44  | BK    | 50      | ASP  | 9.1  |
| 35  | BA    | 654(D)  | G    | 9.0  |
| 35  | DA    | 654(K)  | C    | 8.8  |
| 35  | DA    | 654(G)  | C    | 8.4  |
| 35  | DA    | 654(F)  | C    | 8.3  |
| 30  | B5    | 60      | VAL  | 8.3  |
| 35  | BA    | 654(E)  | G    | 8.2  |
| 35  | BA    | 2802    | G    | 8.2  |
| 11  | CK    | 129     | SER  | 8.0  |
| 30  | B5    | 59      | GLU  | 7.9  |
| 44  | BK    | 11      | GLN  | 7.9  |
| 44  | DK    | 51      | ALA  | 7.8  |
| 1   | CA    | 1030(B) | C    | 7.8  |
| 33  | D8    | 65      | GLU  | 7.8  |
| 22  | AW    | 1       | C    | 7.4  |
| 44  | DK    | 11      | GLN  | 7.3  |

Continued on next page...



*Continued from previous page...*

| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 35  | BA    | 654(J)  | A    | 7.2  |
| 35  | BA    | 2897    | U    | 7.2  |
| 1   | CA    | 1030(A) | G    | 7.1  |
| 35  | BA    | 654(L)  | G    | 7.1  |
| 30  | D5    | 60      | VAL  | 6.9  |
| 35  | DA    | 2897    | U    | 6.9  |
| 35  | BA    | 654(H)  | G    | 6.9  |
| 1   | AA    | 1029    | C    | 6.9  |
| 41  | BG    | 49      | ASP  | 6.8  |
| 44  | BK    | 51      | ALA  | 6.7  |
| 1   | AA    | 1028    | C    | 6.6  |
| 35  | BA    | 2795    | G    | 6.5  |
| 44  | BK    | 61      | ALA  | 6.5  |
| 24  | CY    | 42      | ILE  | 6.5  |
| 1   | AA    | 1030(A) | G    | 6.4  |
| 24  | AY    | 41      | LYS  | 6.4  |
| 25  | D0    | 6       | GLY  | 6.3  |
| 44  | DK    | 52      | ILE  | 6.3  |
| 44  | DK    | 9       | LYS  | 6.2  |
| 52  | BT    | 137     | LYS  | 6.2  |
| 44  | DK    | 16      | LYS  | 6.2  |
| 30  | D5    | 59      | GLU  | 6.2  |
| 1   | CA    | 88      | A    | 6.0  |
| 35  | DA    | 2802    | G    | 6.0  |
| 40  | BF    | 12      | LEU  | 6.0  |
| 35  | DA    | 654(H)  | G    | 5.9  |
| 35  | DA    | 654(I)  | C    | 5.9  |
| 57  | DY    | 107     | ASP  | 5.9  |
| 35  | DA    | 2796    | U    | 5.9  |
| 24  | CY    | 116     | PRO  | 5.8  |
| 35  | DA    | 654(S)  | G    | 5.8  |
| 41  | BG    | 48      | GLU  | 5.7  |
| 57  | DY    | 28      | LYS  | 5.7  |
| 35  | BA    | 654(C)  | G    | 5.7  |
| 40  | DF    | 1       | MET  | 5.6  |
| 13  | CM    | 126     | LYS  | 5.6  |
| 37  | DC    | 147     | GLY  | 5.6  |
| 35  | BA    | 654(G)  | C    | 5.6  |
| 41  | DG    | 48      | GLU  | 5.6  |
| 44  | DK    | 26      | ALA  | 5.5  |
| 24  | AY    | 116     | PRO  | 5.5  |
| 25  | D0    | 5       | LYS  | 5.5  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 32  | B7    | 49      | ARG  | 5.5  |
| 44  | DK    | 50      | ASP  | 5.4  |
| 24  | AY    | 43      | GLY  | 5.4  |
| 13  | CM    | 122     | LYS  | 5.4  |
| 1   | CA    | 1035    | A    | 5.4  |
| 44  | DK    | 2       | LYS  | 5.2  |
| 1   | CA    | 82      | U    | 5.2  |
| 1   | AA    | 1030(C) | G    | 5.2  |
| 25  | B0    | 4       | LYS  | 5.2  |
| 44  | DK    | 18      | THR  | 5.1  |
| 40  | BF    | 8       | GLN  | 5.1  |
| 1   | CA    | 1026    | G    | 5.1  |
| 44  | BK    | 15      | GLY  | 5.1  |
| 22  | CW    | 1       | C    | 5.0  |
| 44  | DK    | 27      | LEU  | 5.0  |
| 44  | DK    | 3       | LYS  | 5.0  |
| 1   | CA    | 81      | U    | 4.8  |
| 25  | D0    | 3       | HIS  | 4.8  |
| 44  | BK    | 7       | VAL  | 4.8  |
| 44  | BK    | 17      | ALA  | 4.8  |
| 44  | BK    | 63      | ARG  | 4.8  |
| 1   | AA    | 81      | U    | 4.8  |
| 44  | DK    | 10      | LEU  | 4.7  |
| 35  | DA    | 654(L)  | G    | 4.7  |
| 44  | DK    | 65      | PHE  | 4.7  |
| 30  | B5    | 58      | LEU  | 4.6  |
| 44  | BK    | 60      | TYR  | 4.6  |
| 57  | DY    | 106     | LEU  | 4.6  |
| 1   | AA    | 1031    | G    | 4.6  |
| 29  | D4    | 57      | GLU  | 4.5  |
| 44  | BK    | 97      | GLY  | 4.5  |
| 13  | CM    | 125     | ARG  | 4.5  |
| 24  | CY    | 64      | THR  | 4.5  |
| 25  | D0    | 7       | LEU  | 4.5  |
| 25  | D0    | 8       | GLY  | 4.5  |
| 37  | DC    | 116     | ALA  | 4.4  |
| 24  | CY    | 690     | GLY  | 4.4  |
| 35  | DA    | 1174    | A    | 4.4  |
| 24  | AY    | 113     | GLY  | 4.4  |
| 24  | AY    | 114     | VAL  | 4.4  |
| 44  | DK    | 55      | VAL  | 4.4  |
| 35  | BA    | 275     | G    | 4.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 44  | DK    | 20   | ALA  | 4.4  |
| 44  | DK    | 54   | PRO  | 4.4  |
| 37  | DC    | 79   | ALA  | 4.3  |
| 40  | DF    | 133  | ASN  | 4.3  |
| 44  | BK    | 31   | GLY  | 4.3  |
| 44  | DK    | 22   | PRO  | 4.3  |
| 44  | BK    | 83   | GLY  | 4.3  |
| 40  | BF    | 25   | PRO  | 4.3  |
| 52  | BT    | 136  | GLN  | 4.2  |
| 35  | DA    | 2793 | G    | 4.2  |
| 40  | DF    | 208  | GLY  | 4.2  |
| 37  | DC    | 78   | ILE  | 4.2  |
| 44  | BK    | 32   | ALA  | 4.1  |
| 44  | DK    | 21   | PRO  | 4.1  |
| 12  | CL    | 128  | ALA  | 4.1  |
| 41  | BG    | 50   | ALA  | 4.1  |
| 35  | BA    | 2896 | C    | 4.0  |
| 27  | B2    | 72   | ALA  | 4.0  |
| 35  | DA    | 2896 | C    | 4.0  |
| 39  | DE    | 205  | ALA  | 4.0  |
| 2   | CB    | 7    | VAL  | 4.0  |
| 24  | CY    | 4    | LYS  | 4.0  |
| 25  | D0    | 4    | LYS  | 4.0  |
| 52  | DT    | 135  | ALA  | 4.0  |
| 28  | D3    | 1    | MET  | 3.9  |
| 1   | CA    | 80   | G    | 3.9  |
| 51  | DS    | 109  | GLY  | 3.9  |
| 37  | BC    | 2    | PRO  | 3.9  |
| 44  | BK    | 35   | MET  | 3.9  |
| 44  | BK    | 64   | SER  | 3.9  |
| 48  | DP    | 149  | GLU  | 3.9  |
| 13  | CM    | 123  | ALA  | 3.9  |
| 5   | CE    | 154  | GLY  | 3.9  |
| 1   | AA    | 88   | A    | 3.8  |
| 44  | BK    | 62   | ASP  | 3.8  |
| 44  | BK    | 49   | GLY  | 3.8  |
| 31  | B6    | 42   | TRP  | 3.8  |
| 5   | AE    | 155  | GLU  | 3.8  |
| 44  | BK    | 12   | LEU  | 3.8  |
| 44  | BK    | 47   | ASN  | 3.8  |
| 44  | BK    | 18   | THR  | 3.8  |
| 44  | DK    | 74   | ALA  | 3.8  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 13  | CM    | 124    | PRO  | 3.7  |
| 44  | BK    | 2      | LYS  | 3.7  |
| 37  | DC    | 97     | GLY  | 3.7  |
| 24  | CY    | 41     | LYS  | 3.7  |
| 35  | DA    | 157    | U    | 3.7  |
| 44  | BK    | 14     | ALA  | 3.7  |
| 40  | DF    | 17     | ARG  | 3.6  |
| 25  | B0    | 8      | GLY  | 3.6  |
| 35  | BA    | 2794   | C    | 3.6  |
| 44  | BK    | 66     | THR  | 3.6  |
| 44  | BK    | 82     | ALA  | 3.6  |
| 35  | DA    | 654(C) | G    | 3.6  |
| 13  | AM    | 7      | VAL  | 3.6  |
| 50  | DR    | 2      | ARG  | 3.6  |
| 7   | AG    | 84     | ASN  | 3.6  |
| 48  | BP    | 87     | ASP  | 3.6  |
| 52  | DT    | 137    | LYS  | 3.6  |
| 44  | BK    | 52     | ILE  | 3.6  |
| 11  | AK    | 129    | SER  | 3.6  |
| 40  | BF    | 1      | MET  | 3.6  |
| 44  | DK    | 36     | GLU  | 3.5  |
| 44  | DK    | 37     | PHE  | 3.5  |
| 44  | BK    | 8      | VAL  | 3.5  |
| 25  | B0    | 6      | GLY  | 3.5  |
| 44  | BK    | 22     | PRO  | 3.5  |
| 54  | DV    | 48     | GLY  | 3.5  |
| 44  | DK    | 141    | ALA  | 3.5  |
| 35  | DA    | 275    | G    | 3.5  |
| 13  | AM    | 122    | LYS  | 3.5  |
| 51  | DS    | 61     | ASN  | 3.4  |
| 13  | AM    | 125    | ARG  | 3.4  |
| 29  | D4    | 32     | TYR  | 3.4  |
| 44  | BK    | 27     | LEU  | 3.4  |
| 44  | DK    | 13     | PRO  | 3.4  |
| 13  | CM    | 120    | LYS  | 3.4  |
| 18  | CR    | 88     | LYS  | 3.4  |
| 44  | BK    | 37     | PHE  | 3.4  |
| 1   | AA    | 1035   | A    | 3.4  |
| 44  | DK    | 17     | ALA  | 3.4  |
| 37  | DC    | 124    | VAL  | 3.4  |
| 40  | BF    | 24     | LEU  | 3.4  |
| 1   | AA    | 82     | U    | 3.4  |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 44         | BK           | 65         | PHE         | 3.4         |
| 44         | BK           | 13         | PRO         | 3.3         |
| 1          | CA           | 1001(A)    | G           | 3.3         |
| 24         | CY           | 84         | THR         | 3.3         |
| 39         | BE           | 76         | ARG         | 3.3         |
| 54         | DV           | 36         | PRO         | 3.3         |
| 25         | B0           | 3          | HIS         | 3.3         |
| 13         | CM           | 7          | VAL         | 3.3         |
| 44         | BK           | 36         | GLU         | 3.3         |
| 44         | DK           | 61         | ALA         | 3.2         |
| 37         | DC           | 96         | GLY         | 3.2         |
| 51         | BS           | 60         | GLY         | 3.2         |
| 44         | BK           | 30         | HIS         | 3.2         |
| 35         | DA           | 2799       | C           | 3.2         |
| 44         | DK           | 118        | THR         | 3.2         |
| 35         | DA           | 2804       | C           | 3.2         |
| 52         | DT           | 39         | ARG         | 3.2         |
| 37         | DC           | 98         | GLU         | 3.2         |
| 48         | DP           | 150        | ALA         | 3.1         |
| 35         | DA           | 2795       | G           | 3.1         |
| 24         | CY           | 40         | HIS         | 3.1         |
| 29         | B4           | 47         | GLN         | 3.1         |
| 44         | BK           | 21         | PRO         | 3.1         |
| 44         | BK           | 84         | LEU         | 3.1         |
| 35         | BA           | 2894       | G           | 3.1         |
| 40         | BF           | 133        | ASN         | 3.1         |
| 7          | CG           | 82         | GLY         | 3.1         |
| 41         | DG           | 113        | ARG         | 3.1         |
| 1          | AA           | 1030(D)    | A           | 3.1         |
| 44         | DK           | 30         | HIS         | 3.1         |
| 58         | DZ           | 159        | PRO         | 3.1         |
| 39         | DE           | 204        | ALA         | 3.1         |
| 1          | AA           | 1027       | C           | 3.1         |
| 44         | DK           | 4          | VAL         | 3.1         |
| 35         | DA           | 156        | U           | 3.1         |
| 51         | DS           | 57         | LYS         | 3.1         |
| 9          | CI           | 95         | LYS         | 3.0         |
| 31         | B6           | 26         | ASN         | 3.0         |
| 44         | BK           | 33         | ASN         | 3.0         |
| 44         | DK           | 82         | ALA         | 3.0         |
| 44         | DK           | 137        | GLU         | 3.0         |
| 40         | BF           | 11         | VAL         | 3.0         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 44  | BK    | 69     | THR  | 3.0  |
| 25  | D0    | 2      | ALA  | 3.0  |
| 44  | BK    | 48     | MET  | 3.0  |
| 24  | CY    | 203    | GLU  | 3.0  |
| 35  | BA    | 2796   | U    | 3.0  |
| 24  | CY    | 202    | PRO  | 3.0  |
| 1   | CA    | 1028   | C    | 2.9  |
| 35  | DA    | 654(R) | C    | 2.9  |
| 27  | D2    | 71     | ASN  | 2.9  |
| 19  | AS    | 82     | GLY  | 2.9  |
| 35  | BA    | 2799   | C    | 2.9  |
| 44  | BK    | 28     | GLY  | 2.9  |
| 19  | CS    | 82     | GLY  | 2.9  |
| 51  | DS    | 59     | LYS  | 2.9  |
| 40  | DF    | 23     | ASP  | 2.9  |
| 35  | BA    | 888    | C    | 2.9  |
| 44  | BK    | 41     | PHE  | 2.9  |
| 13  | AM    | 124    | PRO  | 2.9  |
| 35  | DA    | 1534   | U    | 2.9  |
| 44  | DK    | 19     | PRO  | 2.8  |
| 37  | DC    | 80     | LYS  | 2.8  |
| 46  | BN    | 68     | GLU  | 2.8  |
| 44  | BK    | 45     | THR  | 2.8  |
| 19  | CS    | 81     | ARG  | 2.8  |
| 40  | BF    | 10     | PRO  | 2.8  |
| 41  | BG    | 115    | ARG  | 2.8  |
| 44  | BK    | 10     | LEU  | 2.8  |
| 44  | BK    | 67     | PHE  | 2.8  |
| 30  | D5    | 2      | ALA  | 2.8  |
| 24  | AY    | 115    | GLU  | 2.8  |
| 24  | CY    | 17     | ILE  | 2.8  |
| 24  | AY    | 40     | HIS  | 2.8  |
| 24  | CY    | 114    | VAL  | 2.8  |
| 10  | CJ    | 88     | LEU  | 2.8  |
| 42  | BH    | 42     | ARG  | 2.8  |
| 12  | CL    | 129    | ALA  | 2.8  |
| 40  | BF    | 9      | ILE  | 2.8  |
| 1   | CA    | 1257   | U    | 2.8  |
| 29  | D4    | 56     | VAL  | 2.7  |
| 13  | AM    | 126    | LYS  | 2.7  |
| 1   | AA    | 1030   | C    | 2.7  |
| 30  | D5    | 54     | GLY  | 2.7  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 44  | DK    | 66      | THR  | 2.7  |
| 54  | DV    | 20      | LEU  | 2.7  |
| 44  | BK    | 26      | ALA  | 2.7  |
| 44  | DK    | 67      | PHE  | 2.7  |
| 44  | BK    | 105     | LEU  | 2.7  |
| 10  | AJ    | 85      | LEU  | 2.7  |
| 41  | DG    | 2       | PRO  | 2.7  |
| 41  | DG    | 149     | VAL  | 2.7  |
| 14  | AN    | 2       | ALA  | 2.7  |
| 24  | CY    | 115     | GLU  | 2.7  |
| 44  | BK    | 58      | THR  | 2.7  |
| 29  | D4    | 38      | LYS  | 2.7  |
| 44  | BK    | 6       | ALA  | 2.7  |
| 44  | DK    | 38      | VAL  | 2.6  |
| 42  | BH    | 52      | VAL  | 2.6  |
| 10  | AJ    | 88      | LEU  | 2.6  |
| 37  | BC    | 14      | LYS  | 2.6  |
| 24  | CY    | 227     | ILE  | 2.6  |
| 32  | B7    | 48      | LYS  | 2.6  |
| 42  | BH    | 44      | VAL  | 2.6  |
| 44  | BK    | 68      | VAL  | 2.6  |
| 1   | AA    | 1001(A) | G    | 2.6  |
| 35  | DA    | 2803    | C    | 2.6  |
| 44  | BK    | 110     | GLN  | 2.6  |
| 44  | BK    | 137     | GLU  | 2.6  |
| 35  | DA    | 654     | A    | 2.6  |
| 13  | CM    | 121     | LYS  | 2.6  |
| 24  | CY    | 6       | GLU  | 2.6  |
| 39  | DE    | 69      | LYS  | 2.6  |
| 40  | DF    | 2       | LYS  | 2.6  |
| 44  | DK    | 45      | THR  | 2.5  |
| 44  | BK    | 98      | ARG  | 2.5  |
| 28  | B3    | 1       | MET  | 2.5  |
| 35  | BA    | 2801    | A    | 2.5  |
| 48  | BP    | 150     | ALA  | 2.5  |
| 35  | DA    | 654(A)  | G    | 2.5  |
| 31  | D6    | 42      | TRP  | 2.5  |
| 44  | BK    | 74      | ALA  | 2.5  |
| 24  | AY    | 42      | ILE  | 2.5  |
| 1   | AA    | 80      | G    | 2.5  |
| 44  | DK    | 25      | PRO  | 2.5  |
| 35  | BA    | 614(A)  | U    | 2.5  |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 10         | AJ           | 25         | GLU         | 2.5         |
| 44         | DK           | 62         | ASP         | 2.5         |
| 44         | BK           | 54         | PRO         | 2.5         |
| 37         | DC           | 117        | THR         | 2.5         |
| 29         | D4           | 22         | ILE         | 2.5         |
| 10         | AJ           | 33         | GLN         | 2.5         |
| 52         | DT           | 136        | GLN         | 2.5         |
| 2          | AB           | 122        | PHE         | 2.5         |
| 44         | BK           | 56         | GLU         | 2.5         |
| 37         | DC           | 113        | ALA         | 2.5         |
| 10         | CJ           | 73         | ASP         | 2.5         |
| 1          | CA           | 83         | U           | 2.5         |
| 51         | BS           | 43         | GLU         | 2.5         |
| 35         | DA           | 614(A)     | U           | 2.4         |
| 51         | DS           | 108        | GLY         | 2.4         |
| 9          | AI           | 95         | LYS         | 2.4         |
| 7          | CG           | 83         | ALA         | 2.4         |
| 44         | BK           | 19         | PRO         | 2.4         |
| 48         | DP           | 95         | VAL         | 2.4         |
| 44         | BK           | 53         | VAL         | 2.4         |
| 29         | B4           | 32         | TYR         | 2.4         |
| 24         | CY           | 65         | ILE         | 2.4         |
| 42         | DH           | 176        | ALA         | 2.4         |
| 44         | DK           | 39         | LYS         | 2.4         |
| 29         | B4           | 53         | GLU         | 2.4         |
| 42         | BH           | 137        | ASP         | 2.4         |
| 16         | CP           | 83         | GLU         | 2.4         |
| 24         | CY           | 204        | GLU         | 2.4         |
| 54         | DV           | 101        | GLY         | 2.4         |
| 24         | CY           | 43         | GLY         | 2.4         |
| 39         | BE           | 204        | ALA         | 2.4         |
| 44         | DK           | 63         | ARG         | 2.4         |
| 42         | DH           | 101        | ARG         | 2.4         |
| 50         | BR           | 2          | ARG         | 2.4         |
| 40         | BF           | 23         | ASP         | 2.4         |
| 10         | CJ           | 23         | ILE         | 2.4         |
| 19         | CS           | 22         | LEU         | 2.3         |
| 10         | AJ           | 80         | LYS         | 2.3         |
| 25         | D0           | 85         | ALA         | 2.3         |
| 44         | DK           | 29         | GLN         | 2.3         |
| 44         | DK           | 48         | MET         | 2.3         |
| 35         | DA           | 896        | A           | 2.3         |

*Continued on next page...*



*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 35         | DA           | 1740       | G           | 2.3         |
| 18         | AR           | 88         | LYS         | 2.3         |
| 24         | CY           | 445        | GLU         | 2.3         |
| 54         | BV           | 20         | LEU         | 2.3         |
| 44         | DK           | 14         | ALA         | 2.3         |
| 46         | DN           | 139        | GLU         | 2.3         |
| 13         | AM           | 84         | ILE         | 2.3         |
| 44         | BK           | 57         | ILE         | 2.3         |
| 57         | DY           | 53         | PRO         | 2.3         |
| 2          | AB           | 13         | ALA         | 2.3         |
| 35         | DA           | 884        | C           | 2.3         |
| 42         | BH           | 33         | LEU         | 2.3         |
| 48         | DP           | 5          | ASP         | 2.3         |
| 24         | CY           | 97         | SER         | 2.3         |
| 27         | D2           | 72         | ALA         | 2.3         |
| 1          | AA           | 1037       | C           | 2.3         |
| 44         | DK           | 8          | VAL         | 2.2         |
| 19         | AS           | 81         | ARG         | 2.2         |
| 33         | B8           | 65         | GLU         | 2.2         |
| 26         | B1           | 85         | LEU         | 2.2         |
| 40         | DF           | 194        | MET         | 2.2         |
| 48         | BP           | 81         | GLN         | 2.2         |
| 46         | BN           | 139        | GLU         | 2.2         |
| 25         | D0           | 81         | VAL         | 2.2         |
| 1          | AA           | 470        | C           | 2.2         |
| 38         | DD           | 276        | LYS         | 2.2         |
| 54         | DV           | 1          | MET         | 2.2         |
| 1          | AA           | 93         | G           | 2.2         |
| 35         | BA           | 352        | G           | 2.2         |
| 24         | CY           | 570        | GLY         | 2.2         |
| 34         | D9           | 1          | MET         | 2.2         |
| 40         | DF           | 205        | ARG         | 2.2         |
| 52         | BT           | 135        | ALA         | 2.2         |
| 44         | DK           | 28         | GLY         | 2.2         |
| 39         | BE           | 69         | LYS         | 2.2         |
| 24         | CY           | 401        | SER         | 2.2         |
| 29         | D4           | 58         | ARG         | 2.2         |
| 40         | DF           | 161        | GLU         | 2.2         |
| 42         | BH           | 175        | LYS         | 2.1         |
| 57         | BY           | 28         | LYS         | 2.1         |
| 40         | DF           | 25         | PRO         | 2.1         |
| 35         | BA           | 654(S)     | G           | 2.1         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 44  | DK    | 56   | GLU  | 2.1  |
| 48  | BP    | 149  | GLU  | 2.1  |
| 11  | AK    | 127  | LYS  | 2.1  |
| 42  | DH    | 85   | LYS  | 2.1  |
| 1   | CA    | 1029 | C    | 2.1  |
| 44  | DK    | 23   | VAL  | 2.1  |
| 25  | B0    | 2    | ALA  | 2.1  |
| 44  | DK    | 32   | ALA  | 2.1  |
| 1   | AA    | 1005 | A    | 2.1  |
| 35  | BA    | 654  | A    | 2.1  |
| 2   | AB    | 14   | GLY  | 2.1  |
| 25  | B0    | 7    | LEU  | 2.1  |
| 27  | B2    | 71   | ASN  | 2.1  |
| 35  | BA    | 1174 | A    | 2.1  |
| 28  | D3    | 2    | PRO  | 2.1  |
| 58  | BZ    | 159  | PRO  | 2.1  |
| 44  | BK    | 29   | GLN  | 2.1  |
| 10  | AJ    | 4    | ILE  | 2.1  |
| 35  | BA    | 156  | U    | 2.1  |
| 37  | BC    | 131  | ILE  | 2.1  |
| 44  | BK    | 9    | LYS  | 2.1  |
| 44  | DK    | 110  | GLN  | 2.0  |
| 24  | CY    | 66   | THR  | 2.0  |
| 42  | DH    | 170  | ARG  | 2.0  |
| 44  | BK    | 85   | GLU  | 2.0  |
| 19  | CS    | 21   | GLU  | 2.0  |
| 29  | D4    | 31   | ILE  | 2.0  |
| 44  | DK    | 42   | ASN  | 2.0  |
| 40  | DF    | 181  | LEU  | 2.0  |
| 41  | DG    | 75   | LYS  | 2.0  |
| 24  | AY    | 19   | ALA  | 2.0  |
| 37  | BC    | 203  | GLU  | 2.0  |
| 57  | BY    | 39   | VAL  | 2.0  |
| 40  | DF    | 18   | ARG  | 2.0  |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|-----------------------------|-------|
| 22  | 5MU  | CV    | 54  | 20/22 | 0.97 | 0.11 | -    | 89,92,95,96                 | 0     |
| 22  | 5MU  | AV    | 54  | 20/22 | 0.95 | 0.13 | -    | 82,84,86,86                 | 0     |
| 22  | 5MU  | AW    | 55  | 20/22 | 0.83 | 0.14 | -    | 161,165,168,168             | 0     |
| 22  | 5MU  | CW    | 55  | 20/22 | 0.81 | 0.13 | -    | 178,179,186,186             | 0     |

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|-----------------------------|-------|
| 61  | FUA  | AY    | 702 | 37/37 | 0.90 | 0.43 | 1.99  | 98,102,110,111              | 0     |
| 59  | ZN   | AD    | 301 | 1/1   | 1.00 | 0.28 | 1.61  | 32,32,32,32                 | 0     |
| 59  | ZN   | CD    | 301 | 1/1   | 0.99 | 0.28 | 1.04  | 49,49,49,49                 | 0     |
| 61  | FUA  | CY    | 702 | 37/37 | 0.90 | 0.35 | 0.41  | 102,104,107,109             | 0     |
| 59  | ZN   | B9    | 101 | 1/1   | 0.99 | 0.15 | 0.02  | 62,62,62,62                 | 0     |
| 59  | ZN   | AN    | 101 | 1/1   | 1.00 | 0.16 | -0.23 | 35,35,35,35                 | 0     |
| 59  | ZN   | D9    | 101 | 1/1   | 1.00 | 0.12 | -0.51 | 86,86,86,86                 | 0     |
| 62  | GDP  | AY    | 703 | 28/28 | 0.96 | 0.17 | -0.57 | 78,82,83,84                 | 0     |
| 59  | ZN   | CN    | 101 | 1/1   | 1.00 | 0.16 | -0.86 | 66,66,66,66                 | 0     |
| 59  | ZN   | D4    | 101 | 1/1   | 0.89 | 0.07 | -1.04 | 164,164,164,164             | 0     |
| 59  | ZN   | B4    | 101 | 1/1   | 0.91 | 0.12 | -1.48 | 122,122,122,122             | 0     |
| 62  | GDP  | CY    | 703 | 28/28 | 0.95 | 0.15 | -1.65 | 81,87,94,95                 | 0     |
| 60  | MG   | AY    | 701 | 1/1   | 0.98 | 0.22 | -     | 30,30,30,30                 | 0     |
| 60  | MG   | CY    | 701 | 1/1   | 0.99 | 0.12 | -     | 39,39,39,39                 | 0     |

### 6.5 Other polymers [i](#)

There are no such residues in this entry.